

=> fil reg; d stat que l19; fil capl; d que nos l23
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STRUCTURE FILE UPDATES: 28 JUN 2007 HIGHEST RN 940062-32-8
 DICTIONARY FILE UPDATES: 28 JUN 2007 HIGHEST RN 940062-32-8

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

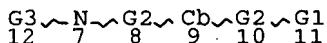
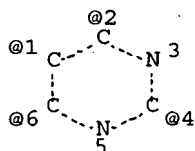
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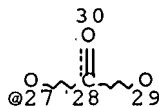
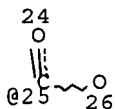
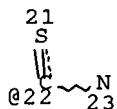
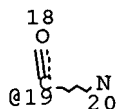
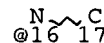
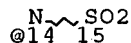
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L3

STR



Ak @13



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REP G2=(0-1) 13

VAR G3=1/2/4/6

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CONNECT IS E2 RC AT 9

CONNECT IS E2 RC AT 13

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GGCAT IS MCY SAT AT 9

GGCAT IS SAT AT 13

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M4-X7 C AT 9

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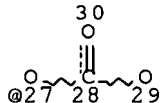
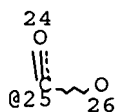
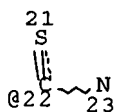
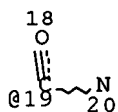
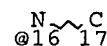
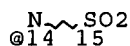
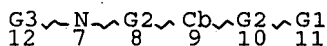
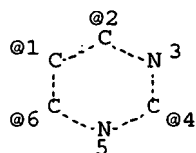
RSPEC 1

NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

L9 563914 SEA FILE=REGISTRY ABB=ON 46.195.39/RID

L16 STR



VAR G1=14/16/19/22/25/27

REP G2=(0-4) C

VAR G3=1/2/4/6

NODE ATTRIBUTES:

NSPEC IS RC AT 17

CONNECT IS E2 RC AT 9

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY SAT AT 9

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M4-X7 C AT 9

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L19 3163 SEA FILE=REGISTRY SUB=L9 SSS FUL (L16 AND L3)

100.0% PROCESSED 563914 ITERATIONS

3163 ANSWERS

SEARCH TIME: 00.00.11

FILE 'CAPLUS' ENTERED AT 09:44:18 ON 29 JUN 2007

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FILE COVERS 1907 - 29 Jun 2007 VOL 147 ISS 2

FILE LAST UPDATED: 28 Jun 2007 (20070628/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

L3 STR
L9 563914 SEA FILE=REGISTRY ABB=ON 46.195.39/RID
L16 STR
L19 3163 SEA FILE=REGISTRY SUB=L9 SSS FUL (L16 AND L3)
L22 77 SEA FILE=CAPLUS ABB=ON L19
L23 39 SEA FILE=CAPLUS ABB=ON L22 AND (PY<2003 OR AY<2003 OR
PRY<2003)

=> d ibib ed abs hitstr l23 1-39; fil hom

L23 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:857175 CAPLUS Full-text
DOCUMENT NUMBER: 141:350167
TITLE: Preparation of imidazolin-2-one derivatives as p38 MAP
kinase inhibitors
INVENTOR(S): Kubo, Akira; Imashiro, Ritsuo; Sakurai, Hiroaki;
Miyoshi, Hidetaka; Ogasawara, Akihito; Hiramatsu,
Hajime; Nakajima, Tatsuo; Nakane, Tetsu
PATENT ASSIGNEE(S): Japan
SOURCE: U.S. Pat. Appl. Publ., 76 pp., Cont.-in-part of Appl.
No. PCT/JP02/10937.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| US 2004204426 | A1 | 20041014 | US 2004-827294 | 20040420 <-- |
| WO 2003035638 | A1 | 20030501 | WO 2002-JP10937 | 20021022 <-- |
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| AU 2004201666 | A1 | 20040513 | AU 2004-201666 | 20040421 <-- |
| WO 2004094404 | A1 | 20041104 | WO 2004-JP5716 | 20040421 |
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SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
TD, TG

JP 2004339210 A 20041202 JP 2004-125060 20040421
EP 1628968 A1 20060301 EP 2004-728708 20040421

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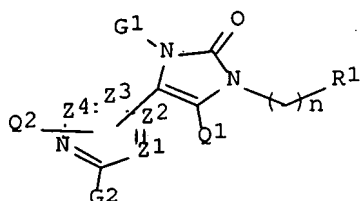
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JP 2002-263680 A 20020910 <--
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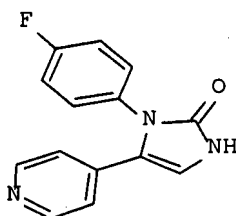
OTHER SOURCE(S): MARPAT 141:350167

ED Entered STN: 18 Oct 2004

GI



I



II

AB The title compds. I [wherein G1 = (un)substituted alkyl or B-W; B = (un)substituted Ph, naphthyl, aromatic heterocyclyl, or cycloalkyl; W = a single bond or (un)substituted alkylene; Q1 and Q2 = independently H, halo, alkyl; n = 0-4; R1 = H, (un)substituted (cyclo)alkyl, Ph, or heterocyclyl; Z1-Z4 = independently CH or N with exclusions; G2 = H, NR3R4, OR5, SR5, COR6, CHR7R8, or heterocyclyl; R3-R8 = independently H, alkenyl, alkynyl, OH, alkoxy, alkoxyoxalyl, alkylsulfonyl, (un)substituted alkyl, amino, alkanoyl, carbamoyl, cycloalkyl, Ph, heterocyclyl(carbonyl), PhCO, or heterocyclyl-CO] and pharmaceutically acceptable salts were prepared as p38 mitogen activation proteins (MAP) kinase inhibitors. Thus, reacting 2,2-diethoxy-2-(pyridin-4-yl)ethylamine (preparation given) with 4-fluorophenyl isocyanate afforded the imidazolinone II. The representative compds. I significantly reduced the production of TNF- α in mice in vivo.

IT 521090-75-5P 521090-76-6P 521091-56-5P
521091-59-8P 521091-62-3P 521091-63-4P
521091-65-6P

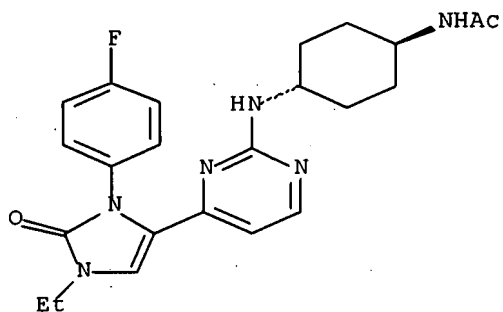
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(MAP kinase inhibitor; preparation of imidazolinones as p38 MAP kinase inhibitors)

RN 521090-75-5 CAPLUS

CN Acetamide, N-[trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI)
(CA INDEX NAME)

Relative stereochemistry.

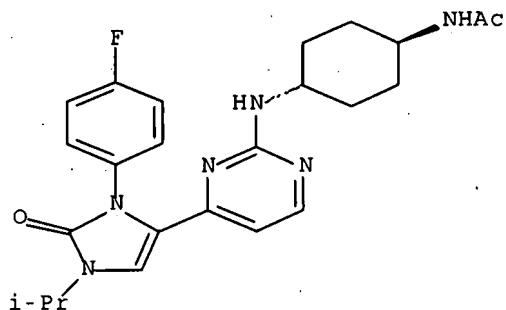


● HCl

RN 521090-76-6 CAPLUS

CN Acetamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

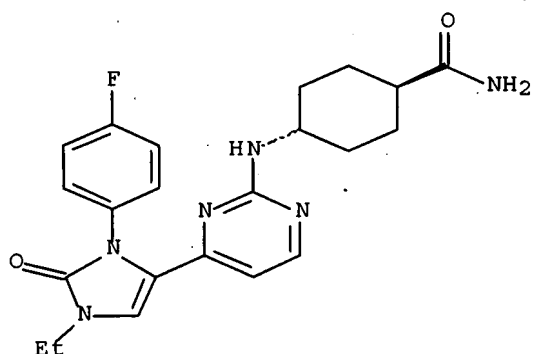


● HCl

RN 521091-56-5 CAPLUS

CN Cyclohexanecarboxamide, 4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

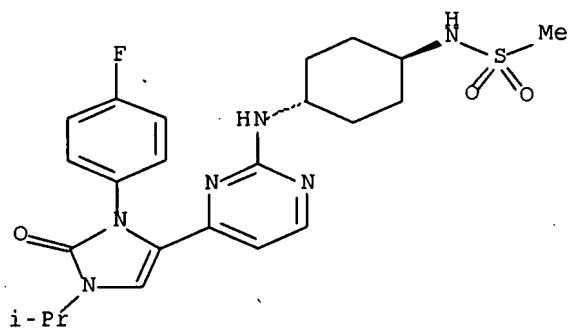


● HCl

RN 521091-59-8 CAPLUS

CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

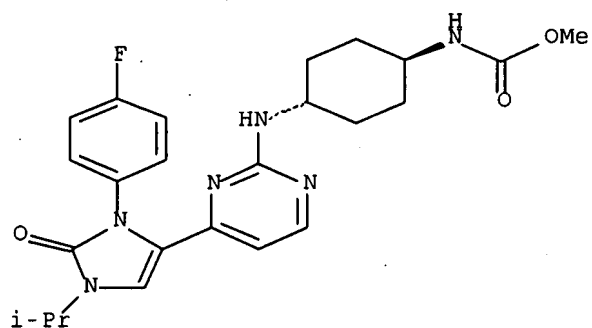


● HCl

RN 521091-62-3 CAPLUS

CN Carbamic acid, [trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

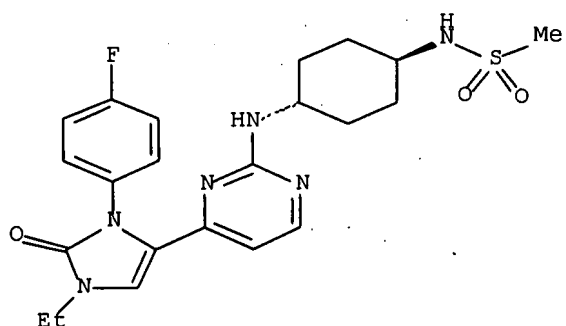


● HCl

RN 521091-63-4 CAPLUS

CN Methanesulfonamide, N-[trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

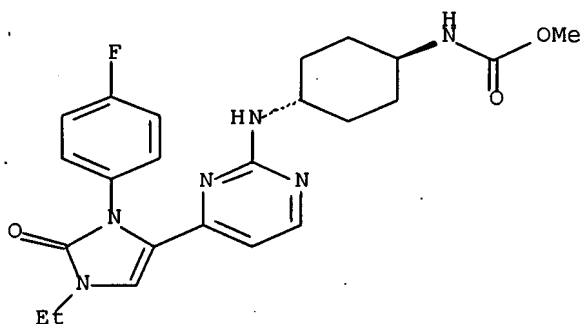


● HCl

RN 521091-65-6 CAPLUS

CN Carbamic acid, [trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

IT 774579-17-8P 774580-02-8P 774580-12-0P
774580-20-0P 774580-26-6P 774580-27-7P
774580-28-8P

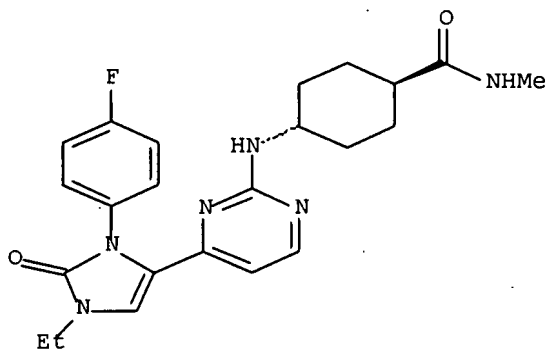
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of imidazolinones as p38 MAP kinase inhibitors)

RN 774579-17-8 CAPLUS

CN Cyclohexanecarboxamide, 4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]-N-methyl-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

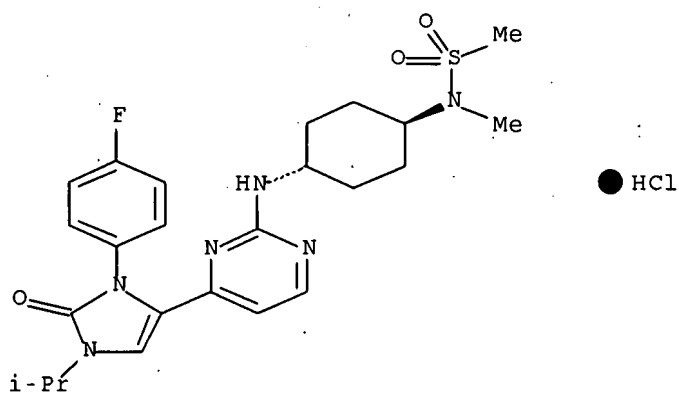


● HCl

RN 774580-02-8 CAPLUS

CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

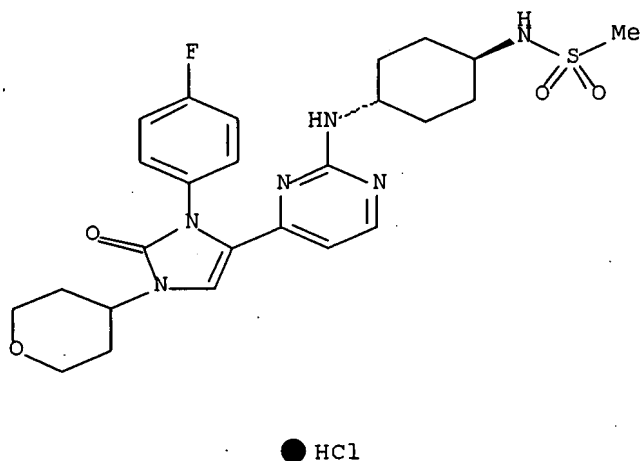
Relative stereochemistry.



RN 774580-12-0 CAPLUS

CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1-(tetrahydro-2H-pyran-4-yl)-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

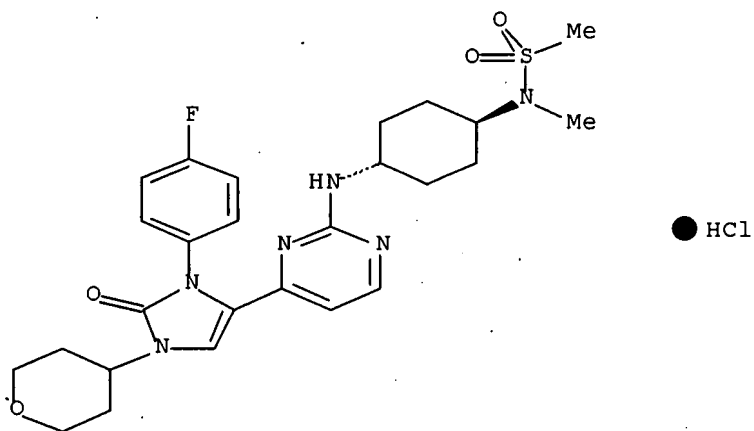
Relative stereochemistry.



RN 774580-20-0 CAPLUS

CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1-(tetrahydro-2H-pyran-4-yl)-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

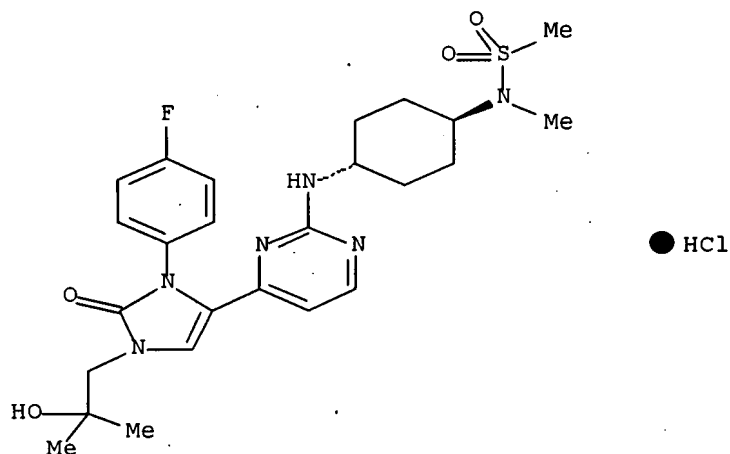
Relative stereochemistry.



RN 774580-26-6 CAPLUS

CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(2-hydroxy-2-methylpropyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

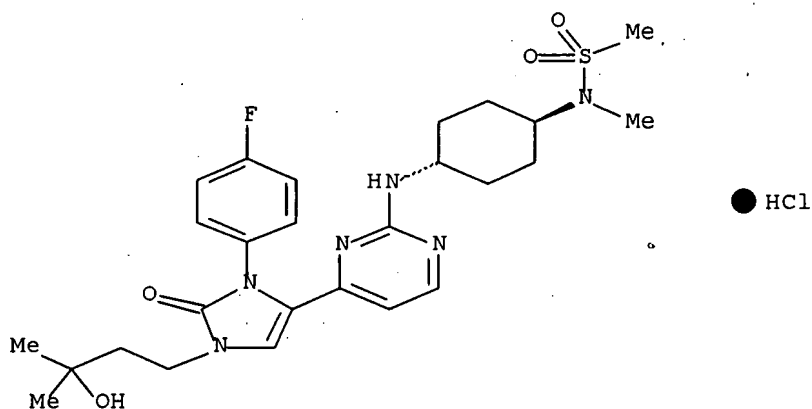
Relative stereochemistry.



RN 774580-27-7 CAPLUS

CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(3-hydroxy-3-methylbutyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

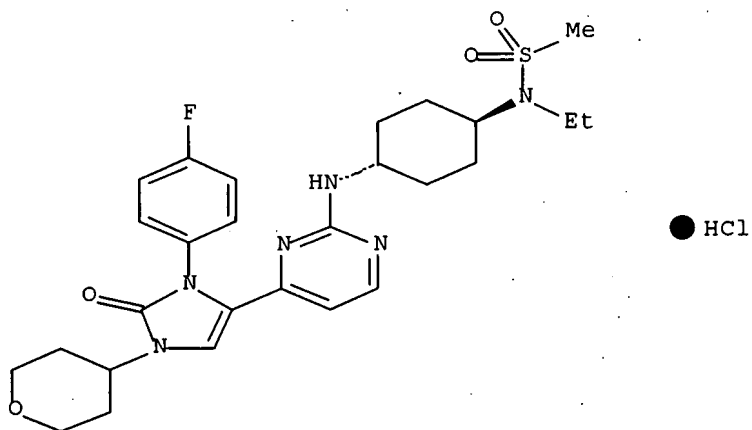
Relative stereochemistry.



RN 774580-28-8 CAPLUS

CN Methanesulfonamide, N-ethyl-N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1-(tetrahydro-2H-pyran-4-yl)-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



L23 ANSWER 2 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:588212 CAPLUS Full-text

DOCUMENT NUMBER: 141:140458

TITLE: Preparation of imidazopyrimidines as tyrosine kinase inhibitors

INVENTOR(S): Hirabayashi, Akihito; Mukoyama, Harunobu; Shiohara, Hiroaki; Kobayashi, Hiroaki; Terao, Yoshihiro; Miyazawa, Keiji; Misawa, Keiko; Onoda, Hideki

PATENT ASSIGNEE(S): Kissei Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 117 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

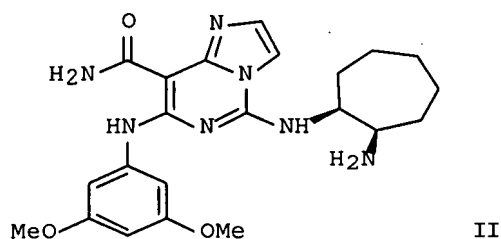
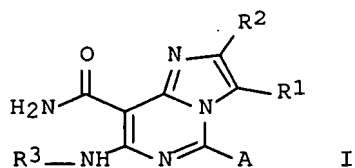
KIND

DATE

APPLICATION NO.

DATE

 JP 2004203748 A 20040722 JP 2002-371196 20021224 <--
 PRIORITY APPLN. INFO.: JP 2002-371196 20021224 <--
 OTHER SOURCE(S): MARPAT 141:140458
 ED Entered STN: 23 Jul 2004
 GI



AB Title compds. I [R1, R2 = H, alkyl, etc.; R3 = H, alkyl, etc.; A = H, alkyl, etc.] were disclosed. In Syk tyrosine kinase inhibition assays, the Ki value of compound II was 1.6 nM. Of note, compds. I have potent inhibition activity against ZAP-70 and/or Syk tyrosine kinase. Compds. I are claimed useful for the treatment of bronchial asthma, allergic rhinitis, etc.

IT 725238-07-3P 725238-09-5P 725238-13-1P
 725238-14-2P 725238-15-3P 725238-16-4P
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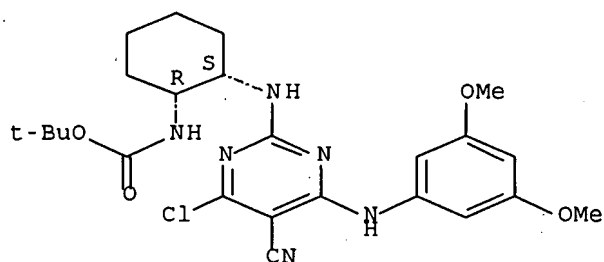
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of imidazopyrimidines as tyrosine kinase inhibitors for treatment of bronchial asthma and allergic dermatitis)

RN 725238-07-3 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-chloro-5-cyano-6-[(3,5-dimethoxyphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

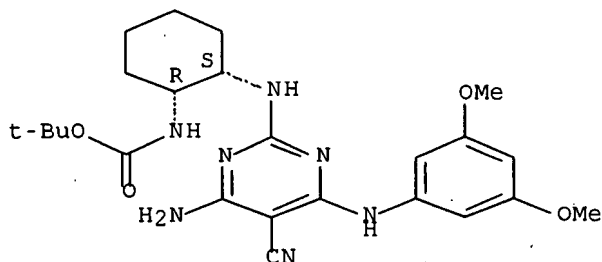
Relative stereochemistry.



RN 725238-09-5 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-cyano-6-[(3,5-dimethoxyphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

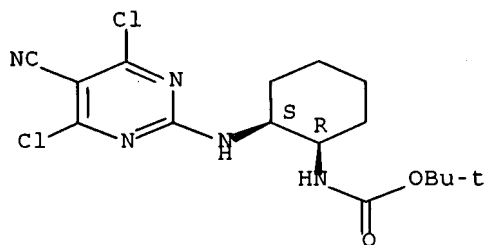
Relative stereochemistry.



RN 725238-13-1 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4,6-dichloro-5-cyano-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

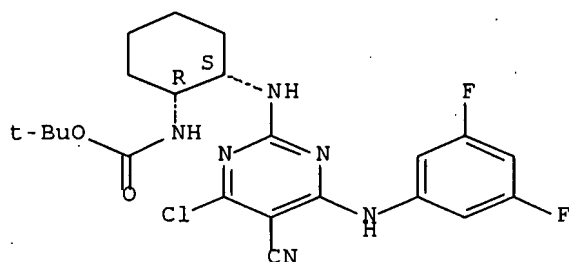
Relative stereochemistry.



RN 725238-14-2 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-chloro-5-cyano-6-[(3,5-difluorophenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

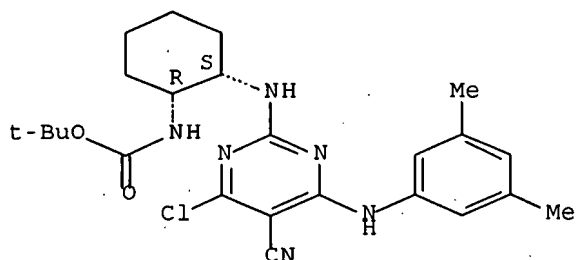
Relative stereochemistry.



RN 725238-15-3 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-chloro-5-cyano-6-[(3,5-dimethylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

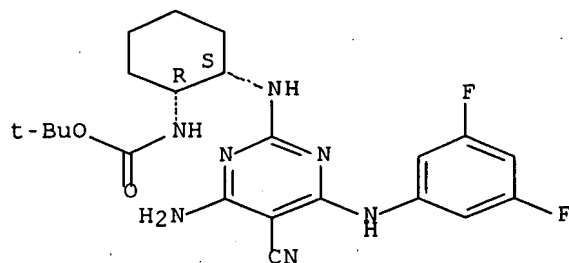
Relative stereochemistry.



RN 725238-16-4 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-cyano-6-[(3,5-difluorophenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

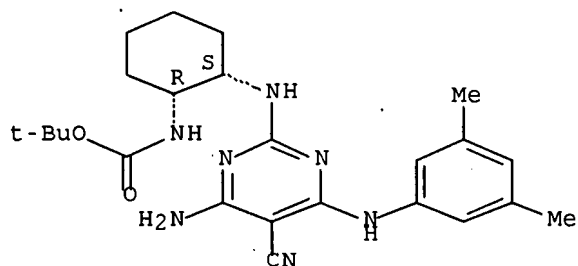
Relative stereochemistry.



RN 725238-17-5 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-cyano-6-[(3,5-dimethylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

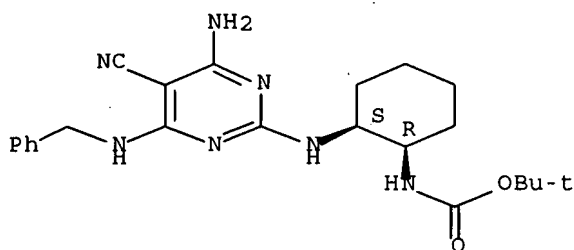
Relative stereochemistry.



RN 725238-18-6 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-cyano-6-[(phenylmethyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

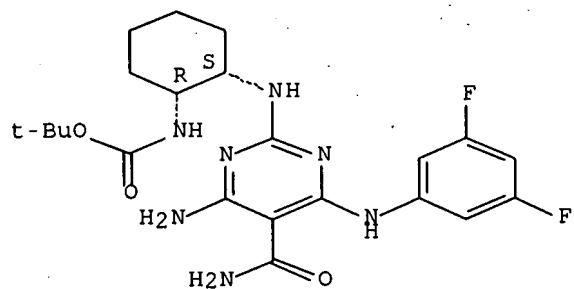
Relative stereochemistry.



RN 725238-19-7 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-(aminocarbonyl)-6-[(3,5-difluorophenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

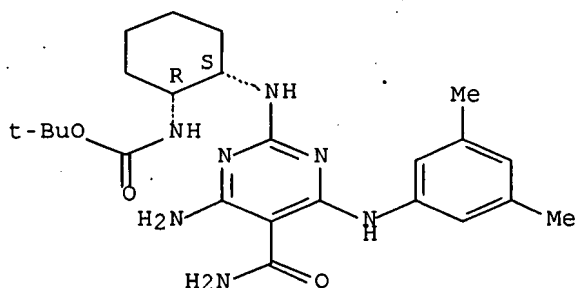
Relative stereochemistry.



RN 725238-20-0 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-(aminocarbonyl)-6-[(3,5-dimethylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

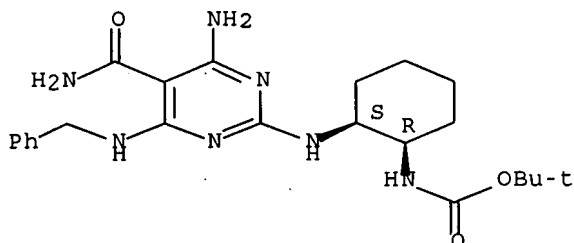
Relative stereochemistry.



RN 725238-21-1 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-(aminocarbonyl)-6-[(phenylmethyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L23 ANSWER 3 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:142963 CAPLUS Full-text

DOCUMENT NUMBER: 140:199334

TITLE: Preparation of 2,4-pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases

INVENTOR(S): Singh, Rajinder; Argade, Ankush; Payan, Donald G.; Clough, Jeffrey; Keim, Holger; Sylvain, Catherine; Li, Hui; Bhamidipati, Somasekhar

PATENT ASSIGNEE(S): Rigel Pharmaceuticals, USA

SOURCE: PCT Int. Appl., 811 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| WO 2004014382 | A1 | 20040219 | WO 2003-US24087 | 20030729 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, | | | | |

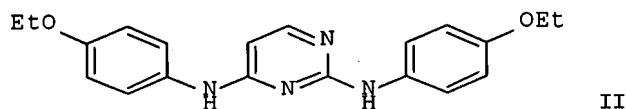
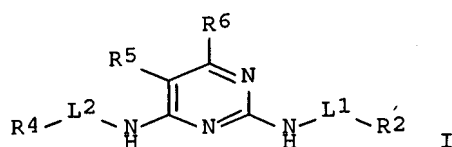
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 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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|--|----|----------|-----------------|----------|--------------|
| CA 2492325 | A1 | 20040219 | CA 2003-2492325 | 20030729 | <-- |
| AU 2003265336 | A1 | 20040225 | AU 2003-265336 | 20030729 | <-- |
| EP 1534286 | A1 | 20050601 | EP 2003-784871 | 20030729 | <-- |
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| BR 2003013059 | A | 20050705 | BR 2003-13059 | 20030729 | <-- |
| CN 1678321 | A | 20051005 | CN 2003-821120 | 20030729 | <-- |
| JP 2006514989 | T | 20060518 | JP 2005-506142 | 20030729 | <-- |
| NZ 537752 | A | 20061222 | NZ 2003-537752 | 20030729 | <-- |
| US 2007060603 | A1 | 20070315 | US 2003-631029 | 20030729 | <-- |
| US 2005038243 | A1 | 20050217 | US 2004-858343 | 20040601 | <-- |
| US 7060827 | B2 | 20060613 | | | |
| US 2005209230 | A1 | 20050922 | US 2004-911684 | 20040803 | <-- |
| SE 2005000203 | A | 20050329 | SE 2005-203 | 20050127 | <-- |
| NO 2005001069 | A | 20050228 | NO 2005-1069 | 20050228 | <-- |
| IN 2005KN00302 | A | 20060421 | IN 2005-KN302 | 20050228 | <-- |
| US 2006025410 | A1 | 20060202 | US 2005-149105 | 20050608 | <-- |
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| US 2006058292 | A1 | 20060316 | US 2005-149418 | 20050608 | <-- |
| US 2006135543 | A1 | 20060622 | US 2005-299207 | 20051208 | <-- |
| PRIORITY APPLN. INFO.: | | | US 2002-399673P | P | 20020729 <-- |
| | | | US 2003-443949P | P | 20030131 |
| | | | US 2003-452339P | P | 20030306 |
| | | | US 2003-631029 | A | 20030729 |
| | | | US 2002-353267P | P | 20020201 <-- |
| | | | US 2002-353333P | P | 20020201 <-- |
| | | | US 2002-434277P | P | 20021217 <-- |
| | | | US 2003-355543 | A1 | 20030131 |
| | | | WO 2003-US24087 | W | 20030729 |
| | | | US 2004-858343 | A3 | 20040601 |

OTHER SOURCE(S): MARPAT 140:199334

ED Entered STN: 22 Feb 2004

GI



AB The present invention provides methods of treating or preventing autoimmune diseases with 2,4-pyrimidinediamine compds., as well as methods of treating, preventing or ameliorating symptoms associated with such diseases. Title compds. I [wherein L1 and L2 = independently a bond or a linker; R2 = (un)substituted alkyl, (hetero)cycloalkyl, or (hetero)aryl; R4 = H or R2; R5 =

R6 or (un)substituted alkyl, alkenyl, or alkynyl; R6 = independently H, an electroneg. group, protected alc. or thiol, haloalkyl(oxy), halo, CN, NC, OCN, SCN, NO, NO₂, N₃, or (un)substituted amino, sulfamoyl(oxy), acyl, carboxy, carbamoyl, (hetero)aryl(alkyl), etc.; with provisos and exclusions; and salts, hydrates, solvates, N-oxides, and prodrugs thereof] were prepared as inhibitors of the IgE and/or IgG receptor signaling cascades that lead to the release of chemical mediators. For example, coupling of 2,4-dichloropyrimidine with 4-ethoxyaniline in EtOH provided N₂,N₄-bis(4-ethoxyphenyl)-2,4-pyrimidinediamine (II). The latter inhibited degranulation of bone marrow derived mast cells challenged with anti-IgE and ionomycin with IC₅₀ values of 4.5 μM and 4.4 μM, resp. Thus, I and their pharmaceutical compns. are useful in the treatment and prevention of diseases characterized by, caused by, or associated with the release of chemical mediators via degranulation of mast, basophil, neutrophil, or eosinophil cells and other processes effected by activation of the IgE and/or IgG receptor signaling cascades. Specific examples of autoimmune diseases that can be treated or prevented with I and their pharmaceutical compns. include rheumatoid arthritis, systemic lupus erythematosus, and multiple sclerosis (no data).

IT 575476-86-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

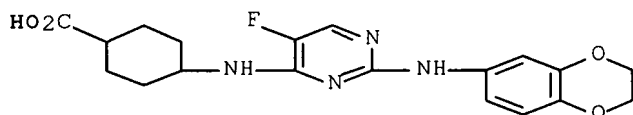
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as

IgE

and/or IgG receptor modulators for treatment of autoimmune diseases)

RN 575476-86-7 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[2-[(2,3-dihydro-1,4-benzodioxin-6-yl)amino]-5-fluoro-4-pyrimidinyl]amino]- (CA INDEX NAME)



IT 575476-87-8

RL: RCT (Reactant); RACT (Reactant or reagent)

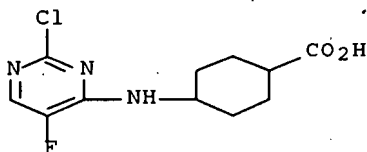
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators

for

treatment of autoimmune diseases)

RN 575476-87-8 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(2-chloro-5-fluoro-4-pyrimidinyl)amino]- (9CI) (CA INDEX NAME)



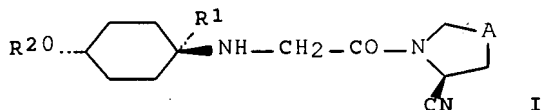
REFERENCE COUNT:

12

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2004:17853 CAPLUS Full-text
 DOCUMENT NUMBER: 140:71039
 TITLE: Pharmaceutical compositions containing aliphatic
 group-containing five-membered nitrogen heterocyclic
 compounds
 INVENTOR(S): Yasuda, Kosuke; Morimoto, Keiji; Kanan, Saburo;
 Hikota, Masaki; Matsumoto, Takeshi; Arakawa, Kenji
 PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 83 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------------------|------|----------|-----------------|----------------|
| JP 2004002368 | A | 20040108 | JP 2003-101362 | 20030404 <-- |
| PRIORITY APPLN. INFO.: | | | JP 2002-102758 | A 20020404 <-- |
| OTHER SOURCE(S): MARPAT 140:71039 | | | | |
| ED Entered STN: 09 Jan 2004 | | | | |
| GI | | | | |



AB Pharmaceutical compns., which inhibit dipeptidyl peptidase IV (DPPIV) and are especially useful for prevention or treatment of type 2 diabetes, contain aliphatic group-containing 5-membered N heterocyclic compds. I [A = CH₂, S; R₁ = H, lower (hydroxy)alkyl, lower alkoxy-lower alkyl; R₂₀ = (substituted) monocyclic or bicyclic heterocyclyl] or their pharmacol. acceptable salts as active ingredients. I-2HCl (R₁ = H, R₂₀ = phthalimido) (preparation given) inhibited DPPIV in human serum with IC₅₀ of 3.8 nM.

IT 412355-56-7P 412355-59-0P 412355-60-3P
 412355-61-4P 412355-75-0P 412355-76-1P
 412355-77-2P 412355-78-3P

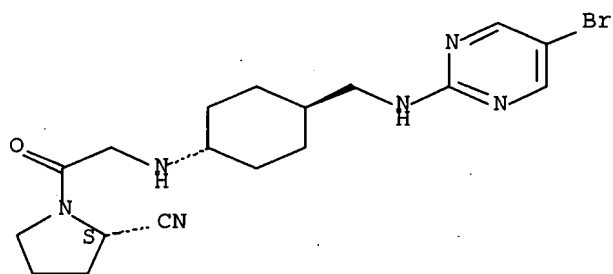
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aliphatic group-containing five-membered nitrogen heterocyclic compds. as dipeptidyl peptidase IV inhibitors for treatment of diabetes, etc.)

RN 412355-56-7 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[[5-bromo-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

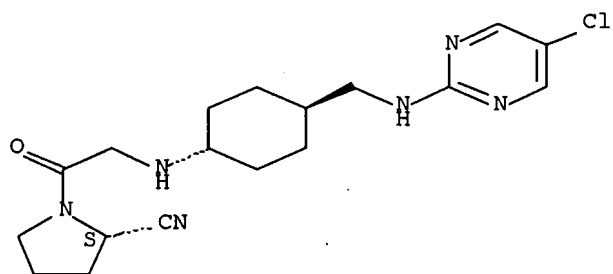


● HCl

RN 412355-59-0 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[[5-chloro-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

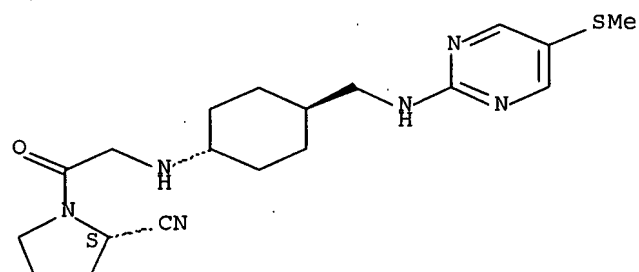


●2 HCl

RN 412355-60-3 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[[5-(methylthio)-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

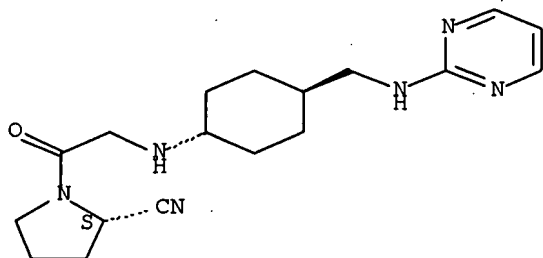


●2 HCl

RN 412355-61-4 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(2-pyrimidinylamino)methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

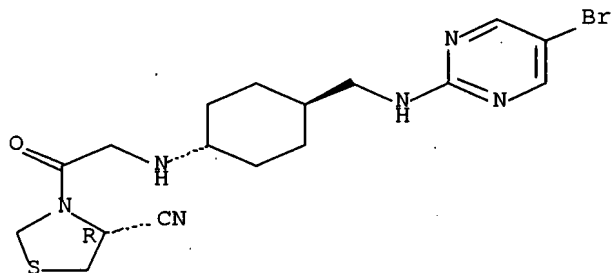


● 2 HCl

RN 412355-75-0 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(5-bromo-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

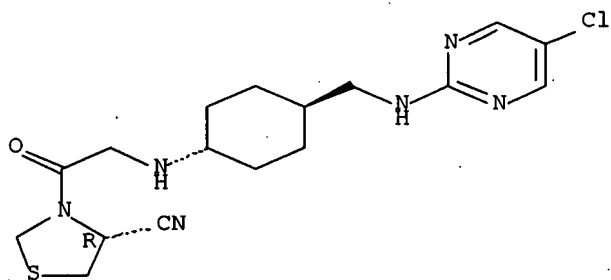


● 2 HCl

RN 412355-76-1 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(5-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

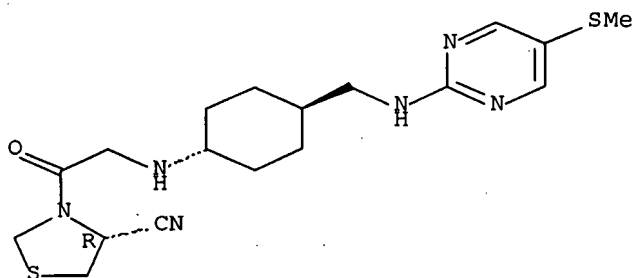


●2 HCl

RN 412355-77-2 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[[5-(methylthio)-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

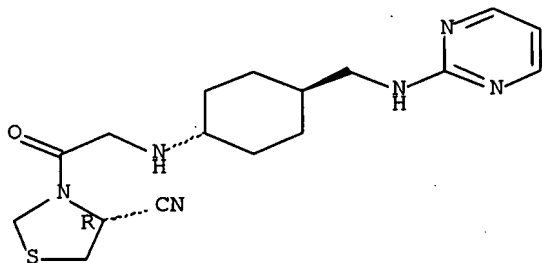


●2 HCl

RN 412355-78-3 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[[2-pyrimidinylamino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

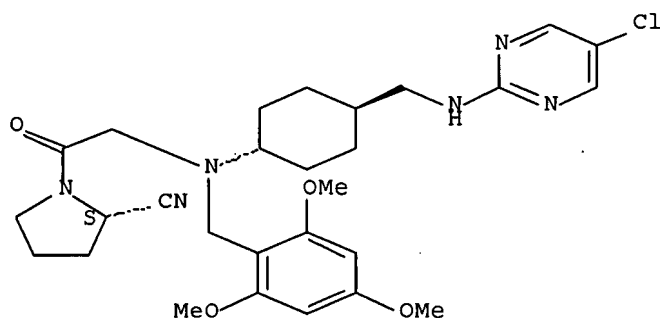
IT 412357-18-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)(preparation of aliphatic group-containing five-membered nitrogen
heterocycliccomps. as dipeptidyl peptidase IV inhibitors for treatment of
diabetes, etc.)

RN 412357-18-7 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[[5-chloro-2-
pyrimidinyl]amino]methyl]cyclohexyl] [(2,4,6-trimethoxyphenyl)methyl]amino]
acetyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L23 ANSWER 5 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:17852 CAPLUS Full-text

DOCUMENT NUMBER: 140:71038

TITLE: Pharmaceutical compositions containing aliphatic
N-containing 5-membered compounds as
dipeptidylpeptidase IV (DPPIV) inhibitorsINVENTOR(S): Yasuda, Kosuke; Morimoto, Keiji; Kanan, Saburo;
Hikota, Masaki; Matsumoto, Takeshi; Arakawa, Kenji

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 129 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

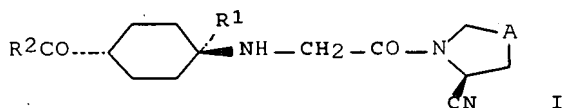
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|-------------|-----------------|----------------|
| JP 2004002367 | A | 20040108 | JP 2003-101361 | 20030404 <-- |
| PRIORITY APPLN. INFO.: | | | JP 2002-102757 | A 20020404 <-- |
| OTHER SOURCE(S): | MARPAT | 140:71038 | | |
| ED Entered STN: | | 09 Jan 2004 | | |

GI



AB The compns., useful for prevention and treatment of type 2 diabetes, contain the compds. I [A = CH₂, S; R₁ = H, lower alkyl, hydroxyalkyl, alkoxyalkyl; R₂ = (un)substituted mono-, di-, or tricyclic hydrocarbyl, heterocyclyl, (un)substituted amino] or their salts. I.HCl (A = CH₂, R₁ = H, R₂ = NMe₂) in vitro inhibited human blood serum DPPIV with IC₅₀ of 3 nM.

IT 412284-89-0P 412284-90-3P 412284-91-4P
 412284-92-5P 412285-02-0P 412285-03-1P
 412285-05-3P 412285-08-6P 412285-09-7P
 412285-11-1P 412285-12-2P 412285-13-3P
 412285-14-4P 412285-15-5P 412285-16-6P
 412285-17-7P 412285-18-8P 412285-19-9P
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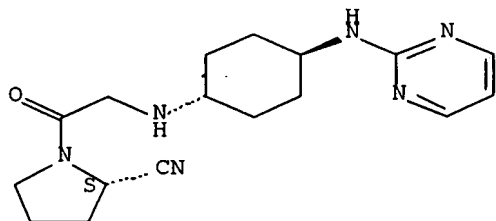
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aliphatic N-containing 5-membered compds. as dipeptidylpeptidase IV inhibitors)

RN 412284-89-0 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

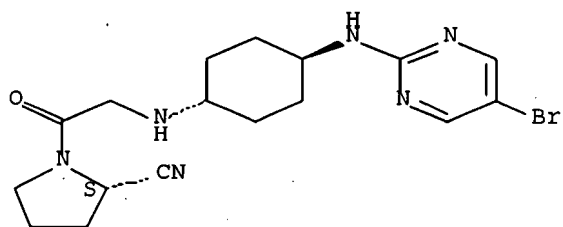


● 2 HCl

RN 412284-90-3 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

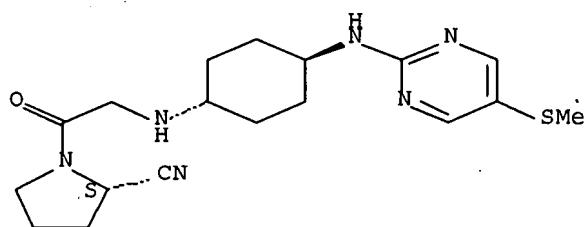


● 2 HCl

RN 412284-91-4 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

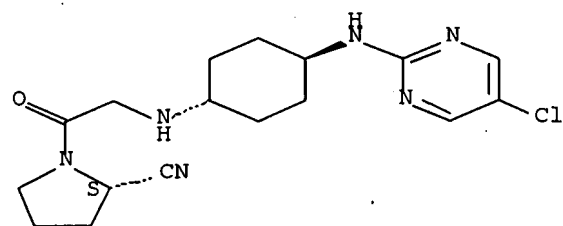


● 2 HCl

RN 412284-92-5 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[5-(chloromethylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

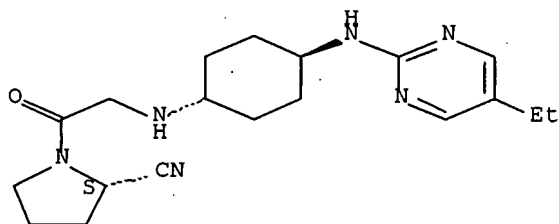


● 2 HCl

RN 412285-02-0 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[5-(ethylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

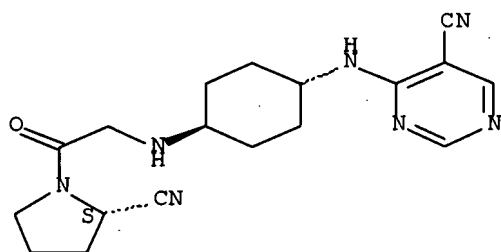


● 2 HCl

RN 412285-03-1 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-cyano-4-ethylpyrimidin-2-yl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

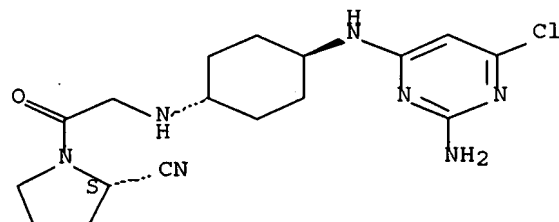


● 2 HCl

RN 412285-05-3 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(2-amino-6-chloro-4-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.



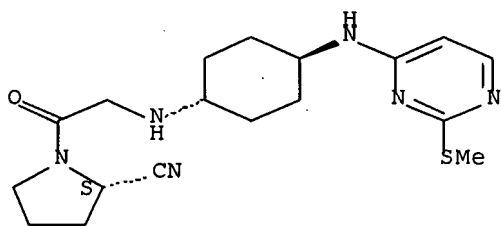
● 2 HCl

RN 412285-08-6 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[2-(methylthio)-4-

pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

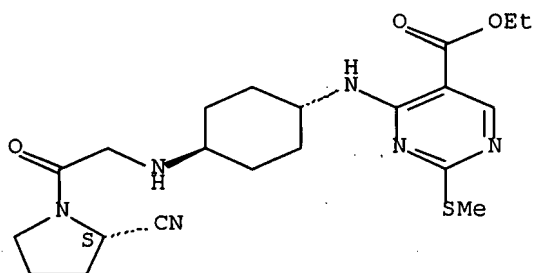


● 2 HCl

RN 412285-09-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(methylthio)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

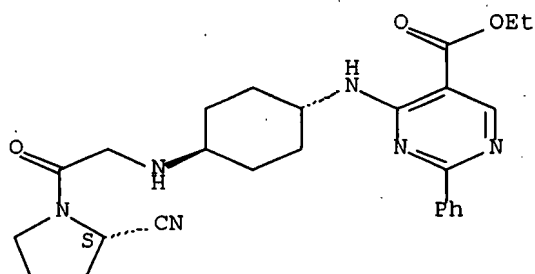


● 2 HCl

RN 412285-11-1 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-phenyl-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

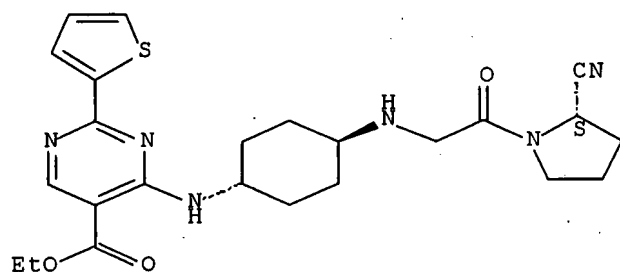


●2 HCl

RN 412285-12-2 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(2-thienyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

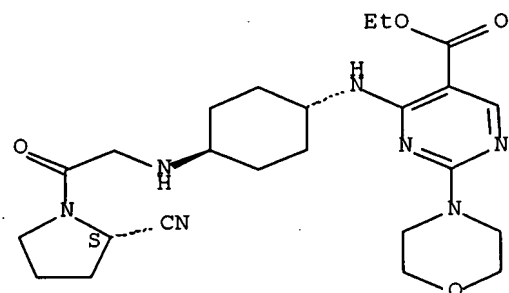


●2 HCl

RN 412285-13-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(4-morpholinyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

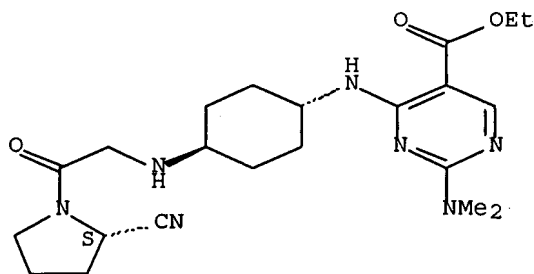


●2 HCl

RN 412285-14-4 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(dimethylamino)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

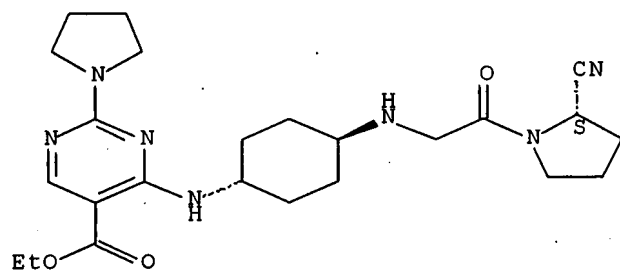


● 2 HCl

RN 412285-15-5 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(1-pyrrolidinyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

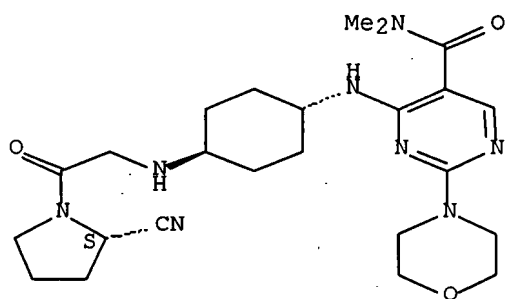


● 2 HCl

RN 412285-16-6 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-N,N-dimethyl-2-(4-morpholinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

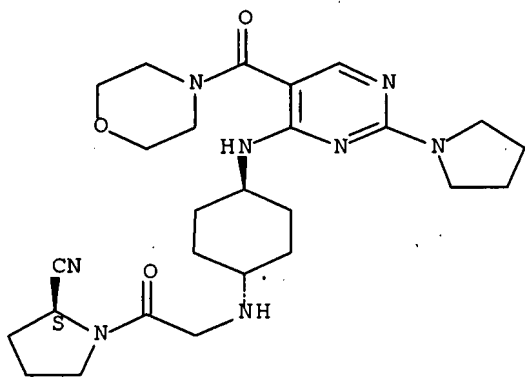


● 2 HCl

RN 412285-17-7 CAPLUS

CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(1-pyrrolidinyl)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

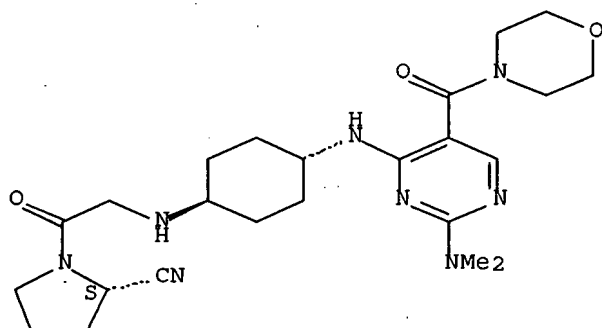


● 2 HCl

RN 412285-18-8 CAPLUS

CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(dimethylamino)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

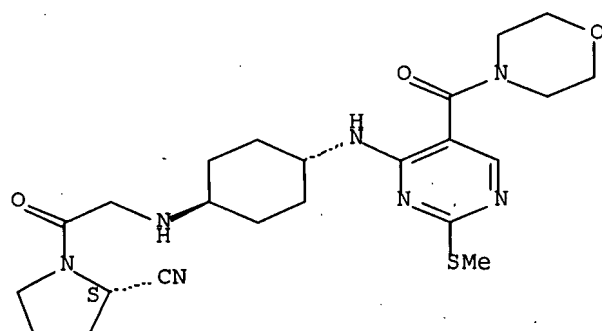


●2 HCl

RN 412285-19-9 CAPLUS

CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(methylthio)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

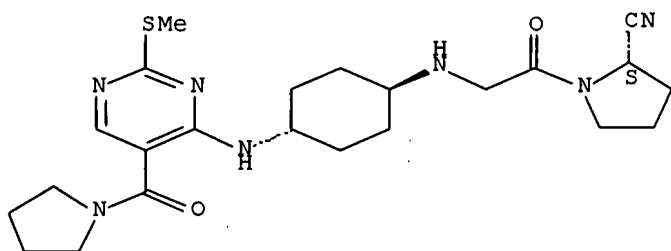


●2 HCl

RN 412285-20-2 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[2-(methylthio)-5-(1-pyrrolidinylcarbonyl)-4-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

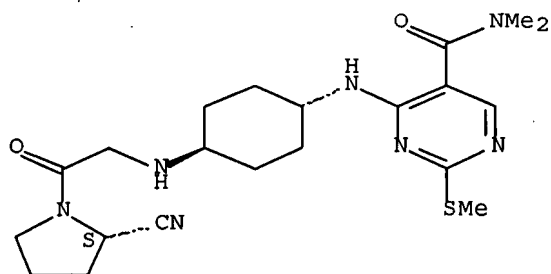


●2 HCl

RN 412285-21-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-[[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-N,N-dimethyl-2-(methylthio)-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

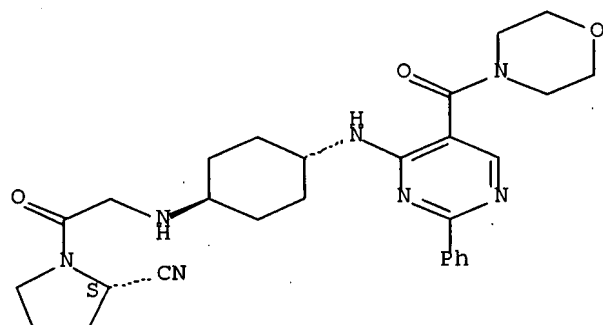


●2 HCl

RN 412285-22-4 CAPLUS

CN Morpholine, 4-[[[4-[[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-phenyl-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

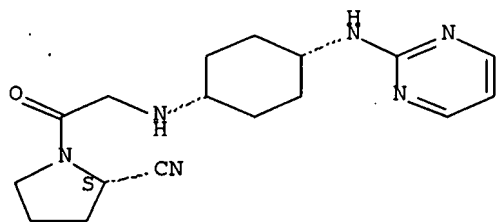


●2 HCl

RN 412285-43-9 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

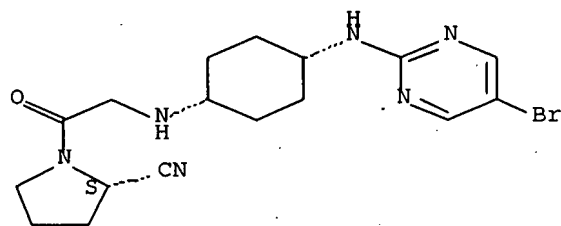


● 2 HCl

RN 412285-44-0 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

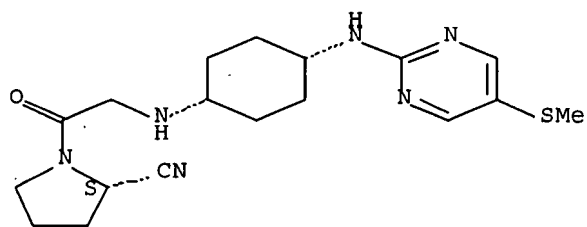


● 2 HCl

RN 412285-45-1 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

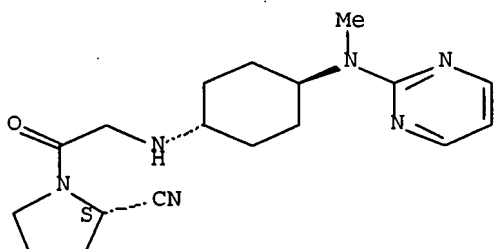


●2 HCl

RN 412285-64-4 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-(methyl-2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

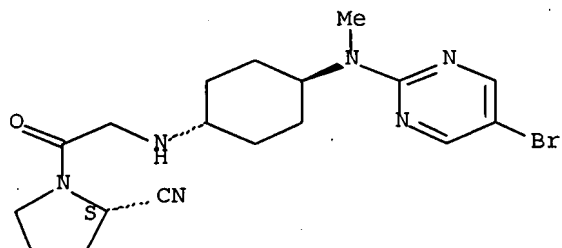


●2 HCl

RN 412285-65-5 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-bromo-2-pyrimidinyl)methylamino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

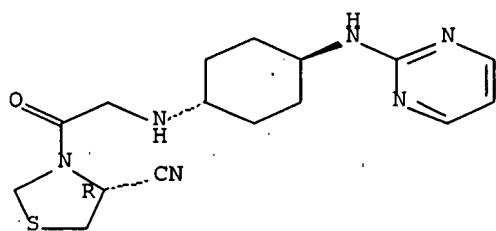


●2 HCl

RN 412288-75-6 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, monohydrochloride, (4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

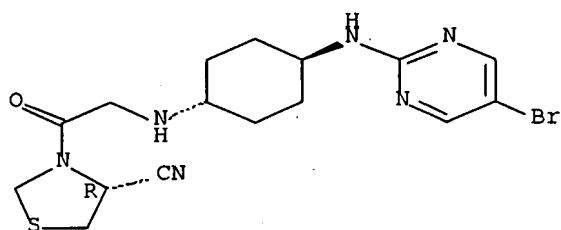


● HCl

RN 412288-76-7 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

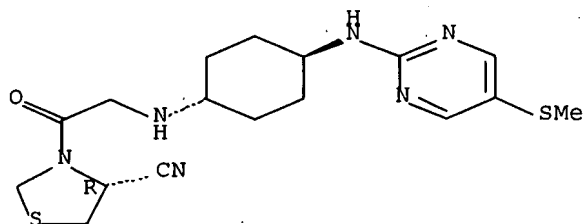


●2 HCl

RN 412288-77-8 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



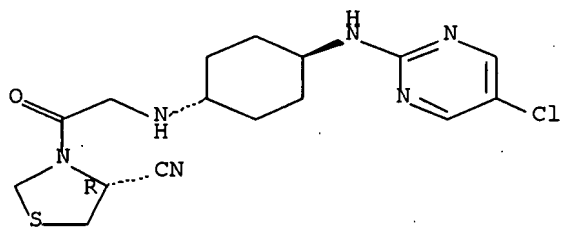
●2 HCl

RN 412288-78-9 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(5-chloro-2-

pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

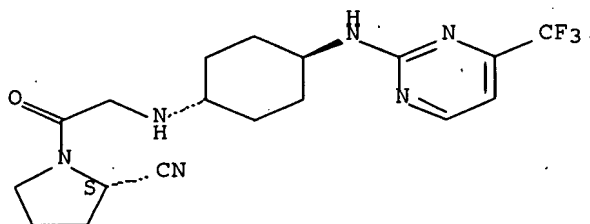


●2 HCl

RN 412915-48-1 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

L23 ANSWER 6 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:971736 CAPLUS Full-text

DOCUMENT NUMBER: 140:16656

TITLE: cis-N-(Quinolin-4-yl)cyclohexane-1,4-diamine derivatives as antagonists of melanin concentrating hormone (MCH) and their pharmaceutical compositions and therapeutic uses, e.g., for treatment of obesity

INVENTOR(S): Kym, Philip R.; Hartandi, Kresna; Gao, Ju; Phelan, Kathleen M.; Akritopoulou-Zanze, Irini; Collins, Christine A.; Vasudevan; Anil; Verzal, Mary K.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: U.S. Pat. Appl. Publ., 89 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

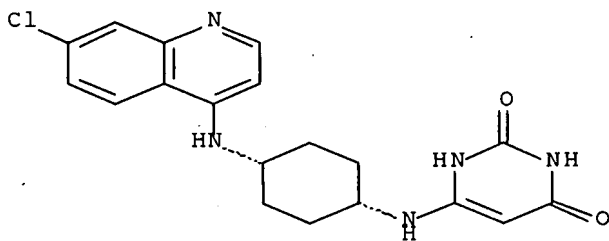
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|-------|-----------------|-------|
| ----- | ---- | ----- | ----- | ----- |

US 2003229119 A1 20031211 US 2003-372359 20030221 <--
 US 6818772 B2 20041116
 PRIORITY APPLN. INFO.: MARPAT 140:16656
 OTHER SOURCE(S):
 ED Entered STN: 14 Dec 2003
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

- AB The invention is directed to the compds. of formula I, or therapeutically suitable salts, esters, prodrugs, or zwitterions thereof [R1, R2, R3 = H, alkyl, alkoxy, halo, haloalkyl, haloalkoxy, OH, NH2 and derivs.; R4 = H, alkyl; R5 = -(CH2)mYAB; m = 0-6; A = bond, alkoxyalkylene, alkylene, or hydroxyalkylene; B = H, alkyl, aryl, aroyl, arylsulfonyl, aralkenyl, aryloxyalkyl, biaryl, biarylalkyl, cycloalkyl, heterocyclyl, heterocyclylcarbonyl, heterocyclylsulfonyl, haloalkyl, NH2 or derivs., carbamoyl or derivs., OH or derivs., SH or derivs.; Y = CO, S, SO, SO2, or bond; R6 = H, alkyl, arylcarboxyalkyl; R7, R8, R9, R10 = H, alkyl, alkoxy, halo, haloalkyl, haloalkoxy, OH; or R7R8 = oxo; with 4 provisos]. The invention further relates to the antagonism of the effects of melanin-concentrating hormone (MCH) through the MCH receptor, which is useful for the prevention or treatment of eating disorders, weight gain, obesity, abnormalities in reproduction and sexual behavior, thyroid hormone secretion, diuresis and water/electrolyte homeostasis, sensory processing, memory, sleeping, arousal, anxiety, depression, seizures, neurodegeneration and psychiatric disorders. Approx. 450 synthetic examples of I are given. For instance, reaction of N-(7-chloroquinolin-4-yl)cyclohexane-1,4-diamine (cis isomer) with 4-chloro-2,8-bis(trifluoromethyl)quinoline in N-methylpyrrolidinone the presence of Et3N at 150° gave title compound II. In a fluorescence assay for release of intracellular Ca++ induced by activation of MCHR, a more preferred group of compds. I inhibited MCH-induced fluorescence in a range of 90-100% at 10 µM. A more preferred group of I also gave 90-100% inhibition of 125I-MCH binding to human MCHR1 at 2 µM (no addnl. data).
- IT 589492-45-5P, cis-6-[[4-[(7-Chloroquinolin-4-yl)amino]cyclohexyl]amino]pyrimidine-2,4(1H,3H)-dione
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of quinolinylcyclohexanediamine derivs. as MCH receptor antagonists)
- RN 589492-45-5 CAPLUS
- CN 2,4(1H,3H)-Pyrimidinedione, 6-[[cis-4-[(7-chloro-4-quinolinyl)amino]cyclohexyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

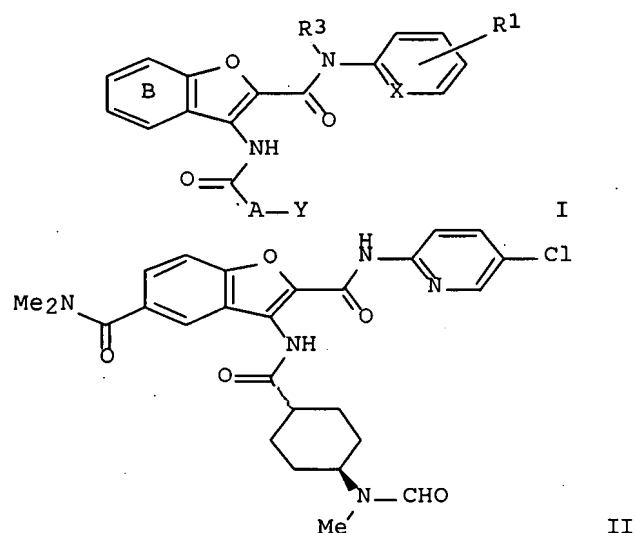


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 7 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:796684 CAPLUS Full-text
 DOCUMENT NUMBER: 139:292142
 TITLE: Preparation of benzofuran derivatives as activated
 blood coagulation factor X inhibitors for treatment of
 thrombosis
 INVENTOR(S): Kawaguchi, Takayuki; Akatsuka, Hidenori; Iijima, Toru;
 Tsuboi, Yasunori; Mitsui, Takashi; Murakami, Jun
 PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 274 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------------|
| WO 2003082847 | A1 | 20031009 | WO 2003-JP3807 | 20030327 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| JP 2004250417 | A | 20040909 | JP 2003-84865 | 20030326 <-- |
| CA 2479831 | A1 | 20031009 | CA 2003-2479831 | 20030327 <-- |
| AU 2003221178 | A1 | 20031013 | AU 2003-221178 | 20030327 <-- |
| EP 1489078 | A1 | 20041222 | EP 2003-712982 | 20030327 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| BR 2003008796 | A | 20050111 | BR 2003-8796 | 20030327 <-- |
| CN 1656086 | A | 20050817 | CN 2003-811791 | 20030327 <-- |
| NZ 535267 | A | 20060331 | NZ 2003-535267 | 20030327 <-- |
| RU 2286344 | C2 | 20061027 | RU 2004-131680 | 20030327 <-- |
| ZA 2004007359 | A | 20050628 | ZA 2004-7359 | 20040914 <-- |
| US 2005282808 | A1 | 20051222 | US 2004-508512 | 20040921 <-- |
| IN 2004CN02112 | A | 20060303 | IN 2004-CN2112 | 20040922 <-- |
| NO 2004004644 | A | 20041216 | NO 2004-4644 | 20041027 <-- |
| PRIORITY APPLN. INFO.: | | | JP 2002-91686 | A 20020328 <-- |
| | | | JP 2002-376158 | A 20021226 <-- |
| | | | WO 2003-JP3807 | W 20030327 |

OTHER SOURCE(S): MARPAT 139:292142
 ED Entered STN: 10 Oct 2003
 GI



AB The title compds. I [wherein X = N or CH; Y = (un)substituted amino, cycloalkyl, or saturated heterocyclyl; A = a single bond, O, or hydrocarbyl; R1 = H, halo, alkyl, alkoxy, CN, or (un)substituted amino; ring B = (un)substituted Ph; R3 = H or alkyl] and pharmaceutically acceptable salts thereof are prepared as activated blood coagulation factor X (FXa) inhibitors. For example, the compound II was prepared in a multi-step synthesis. II showed IC50 of <100 nM against FXa. I are useful for the treatment of thrombosis (no data).

IT 609803-50-1P

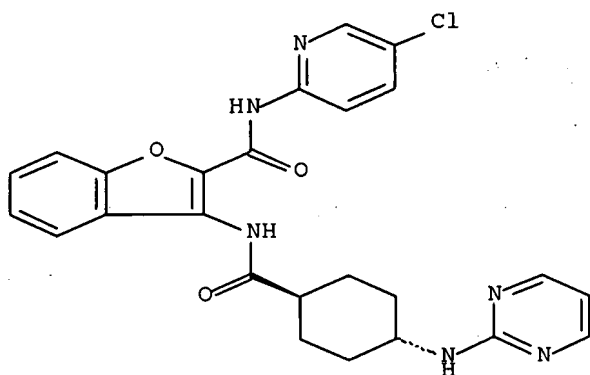
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzofuran derivs. as activated blood coagulation factor X inhibitors for treatment of thrombosis)

RN 609803-50-1 CAPLUS

CN 2-Benzofurancarboxamide, N-(5-chloro-2-pyridinyl)-3-[[[trans-4-(2-pyrimidinylamino)cyclohexyl]carbonyl]amino]-, dihydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



●2 HCl

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 8 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:678662 CAPLUS Full-text
 DOCUMENT NUMBER: 139:214342
 TITLE: cis-N-(Quinolin-4-yl)cyclohexane-1,4-diamine
 derivatives as antagonists of melanin concentrating
 hormone (MCH) and their pharmaceutical compositions
 and therapeutic uses, e.g., for treatment of obesity
 INVENTOR(S): Kym, Philip R.; Hartandi, Kresna; Gao, Ju; Phelan,
 Kathleen M.; Akritopoulou-Zanze, Irini; Collins,
 Christine A.; Vasudevan, Anil; Verzal, Mary K.
 PATENT ASSIGNEE(S): Abbott Laboratories, USA
 SOURCE: PCT Int. Appl., 207 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------------|
| WO 2003070244 | A1 | 20030828 | WO 2003-US5510 | 20030221 <-- |
| W: CA, JP, MX | | | | |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR | | | | |
| PRIORITY APPLN. INFO.: | | | US 2002-81675 | A 20020222 <-- |
| OTHER SOURCE(S): MARPAT 139:214342 | | | | |
| ED Entered STN: 29 Aug 2003 | | | | |
| GI | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention is directed to the compds. of formula I, or therapeutically suitable salts, esters, prodrugs, or zwitterions thereof [R1, R2, R3 = H, alkyl, alkoxy, halo, haloalkyl, haloalkoxy, OH, NH2 and derivs.; R4 = H, alkyl; R5 = -(CH2)mYAB; m = 0-6; A = bond, alkoxyalkylene, alkylene, or hydroxyalkylene; B = H, alkyl, aryl, aroyl, arylsulfonyl, aralkenyl, aryloxyalkyl, biaryl, biarylalkyl, cycloalkyl, heterocyclyl, heterocyclylcarbonyl, heterocyclylsulfonyl, haloalkyl, NH2 or derivs., carbamoyl or derivs., OH or derivs., SH or derivs.; Y = CO, S, SO, SO2, or bond; R6 = H, alkyl, arylcarboxyalkyl; R7, R8, R9, R10 = H, alkyl, alkoxy, halo, haloalkyl, haloalkoxy, OH; or R7R8 = oxo; with 4 provisos]. The invention further relates to the antagonism of the effects of melanin-concentrating hormone (MCH) through the MCH receptor, which is useful for the prevention or treatment of eating disorders, weight gain, obesity, abnormalities in reproduction and sexual behavior, thyroid hormone secretion, diuresis and water/electrolyte homeostasis, sensory processing, memory, sleeping, arousal, anxiety, depression, seizures, neurodegeneration and psychiatric disorders. Approx. 450 synthetic examples of I are given. For instance, reaction of N-(7-chloroquinolin-4-yl)cyclohexane-1,4-diamine (cis isomer) with 4-chloro-2,8-bis(trifluoromethyl)quinoline in N-methylpyrrolidinone the presence of Et3N at 150° gave title compound II. In a fluorescence assay for release of intracellular Ca++ induced by activation of

MCHR, a more preferred group of compds. I inhibited MCH-induced fluorescence in a range of 90-100% at 10 μ M. A more preferred group of I also gave 90-100% inhibition of 125I-MCH binding to human MCHR1 at 2 μ M (no addnl. data).

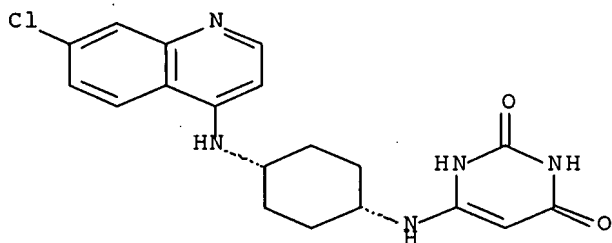
IT 589492-45-5P, cis-6-[[4-[(7-Chloroquinolin-4-yl)amino]cyclohexyl]amino]pyrimidine-2,4(1H,3H)-dione
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of quinolinylcyclohexanedi-amine derivs. as MCH receptor antagonists)

RN 589492-45-5 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-[[cis-4-[(7-chloro-4-quinolinyl)amino]cyclohexyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 9 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:610204 CAPLUS Full-text

DOCUMENT NUMBER: 139:164801

TITLE: Preparation of 2,4-pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction

INVENTOR(S): Singh, Rajinder; Argade, Ankush; Payan, Donald G.; Molineaux, Susan; Holland, Sacha J.; Clough, Jeffrey; Keim, Holger; Bhamidipati, Somasekhar; Sylvain, Catherine; Li, Weigun; Rossi, Alexander B.

PATENT ASSIGNEE(S): Rigel Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 648 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|------|----------|-----------------|--------------|
| WO 2003063794 | A2 | 20030807 | WO 2003-US3022 | 20030131 <-- |
| WO 2003063794 | A3 | 20031204 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2474277 A1 20030807 CA 2003-2474277 20030131 <--
 US 2004029902 A1 20040212 US 2003-355543 20030131 <--
 EP 1471915 A2 20041103 EP 2003-707654 20030131 <--

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

JP 2005516046 T 20050602 JP 2003-563490 20030131 <--
 CN 1625400 A 20050608 CN 2003-803180 20030131 <--
 BR 2003007355 A 20060411 BR 2003-7355 20030131 <--
 US 2005038243 A1 20050217 US 2004-858343 20040601 <--
 US 7060827 B2 20060613
 US 2005209230 A1 20050922 US 2004-911684 20040803 <--
 IN 2004KN01139 A 20060512 IN 2004-KN1139 20040809 <--
 NO 2004003632 A 20041026 NO 2004-3632 20040831 <--
 US 2006025410 A1 20060202 US 2005-149105 20050608 <--
 US 2006035916 A1 20060216 US 2005-148746 20050608 <--
 US 2006058292 A1 20060316 US 2005-149418 20050608 <--
 US 2006135543 A1 20060622 US 2005-299207 20051208 <--

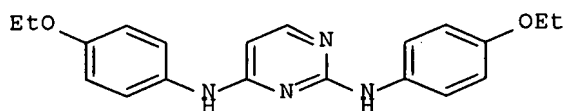
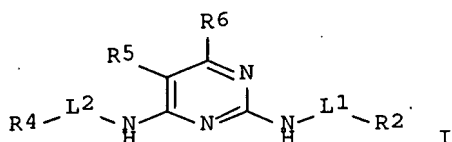
PRIORITY APPLN. INFO.:

US 2002-353267P P 20020201 <--
 US 2002-353333P P 20020201 <--
 US 2002-399673P P 20020729 <--
 US 2002-434277P P 20021217 <--
 US 2003-355543 A1 20030131
 WO 2003-US3022 W 20030131
 US 2004-858343 A3 20040601

OTHER SOURCE(S): MARPAT 139:164801

ED Entered STN: 08 Aug 2003

GI



AB Title compds. I [wherein L1 and L2 = independently a bond or a linker; R2 = (un)substituted alkyl, (hetero)cycloalkyl, or (hetero)aryl; R4 = H or R2; R5 = R6 or (un)substituted alkyl, alkenyl, or alkynyl; R6 = independently H, an electroneg. group, protected alc. or thiol, haloalkyl(oxy), halo, CN, NC, OCN, SCN, NO, NO2, N3, or (un)substituted amino, sulfamoyl(oxy), acyl, carboxy, carbamoyl, (hetero)aryl(alkyl), etc.; with provisos and exclusions; and salts, hydrates, solvates, N-oxides, and prodrugs thereof] were prepared as inhibitors of the IgE and/or IgG receptor signaling cascades that lead to the release of chemical mediators. For example, coupling of 2,4-dichloropyrimidine with 4-ethoxyaniline in EtOH provided N2,N4-bis(4-

ethoxyphenyl)-2,4- pyrimidinediamine (II). The latter inhibited degranulation of bone marrow derived mast cells challenged with anti-IgE and ionomycin with IC50 values of 4.5 μ M and 4.4 μ M, resp. Thus, I and their pharmaceutical compns. are useful in the treatment and prevention of diseases characterized by, caused by, or associated with the release of chemical mediators via degranulation of mast, basophil, neutrophil, or eosinophil cells and other processes effected by activation of the IgE and/or IgG receptor signaling cascades. The treatment and prevention of allergic diseases, low grade scarring, diseases associated with tissue destruction, diseases associated with tissue inflammation, inflammation, and scarring are targeted uses (no data).

IT 575476-86-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

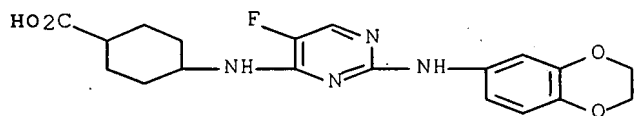
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as

IgE

and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)

RN 575476-86-7 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[2-[(2,3-dihydro-1,4-benzodioxin-6-yl)amino]-5-fluoro-4-pyrimidinyl]amino]- (CA INDEX NAME)



IT 575476-87-8

RL: RCT (Reactant); RACT (Reactant or reagent)

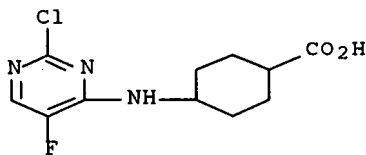
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators

for

treatment of allergic diseases, inflammatory conditions, and tissue destruction)

RN 575476-87-8 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(2-chloro-5-fluoro-4-pyrimidinyl)amino]- (9CI) (CA INDEX NAME)



L23 ANSWER 10 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:532524 CAPLUS Full-text

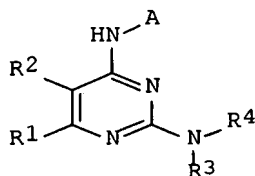
DOCUMENT NUMBER: 139:101141

TITLE: Preparation of 2,4-diaminopyrimidines as inhibitors of prolylpeptidase, inducers of apoptosis and cancer treatment agents

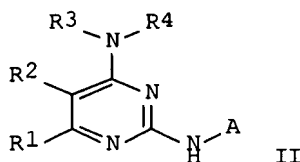
INVENTOR(S): Dumas, Jacques; Dixon, Julie; Sibley, Robert; Wood, Jill

PATENT ASSIGNEE(S): Bayer Corporation, USA
 SOURCE: PCT Int. Appl., 47 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

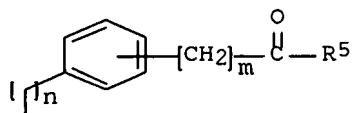
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-------------------|----------------|
| WO 2003055489 | A1 | 20030710 | WO 2002-US41146 | 20021220 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2002367172 | A1 | 20030715 | AU 2002-367172 | 20021220 <-- |
| PRIORITY APPLN. INFO.: | | | US 2001-343047P | P 20011221 <-- |
| | | | WO 2002-US41146 | W 20021220 <-- |
| OTHER SOURCE(S): | | | MARPAT 139:101141 | |
| ED Entered STN: 11 Jul 2003 | | | | |
| GI | | | | |



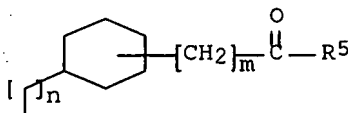
I



II



III



IV

AB The title compds. [I or II; R1, R2 = H, halo, OH, etc.; R3 = H; R4 = (un)substituted alkyl, cycloalkyl, aryl, alkylaryl; or NR3R4 = (un)saturated 4-8 membered heterocyclyl which optionally contains 1-3 addnl. heteroatoms selected from N, O and S; A = III or IV; R5 = OH, OR6, NR8R9; R6 = alkyl, haloalkyl, aryl, haloaryl; R8, R9 = H, alkyl, aryl, etc.; n, m = 0-1], useful for the inhibiting prolylpeptidase, inducing apoptosis and treating cancer, were prepared E.g., a 3-step synthesis of I [A = 4-(HO2C)C6H4CH2; R1 = H; R2 = Me; R3 = H; R4 = 2-thienylmethyl], starting from Me 4-(aminomethyl)benzoate and 2,4-dichloro-5-methylpyrimidine, was given. All exemplified compds. I were found to inhibit prolylpeptidase at or below of 10 μ M.

IT 557789-86-3P 557789-87-4P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

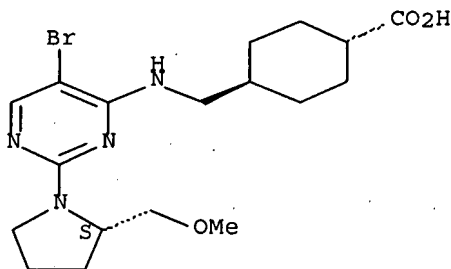
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2,4-diaminopyrimidines as inhibitors of prolylpeptidase, inducers of apoptosis and cancer treatment agents)

RN 557789-86-3 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[5-bromo-2-[(2S)-2-(methoxymethyl)-1-pyrrolidinyl]-4-pyrimidinyl]amino]methyl]-, trans- (9CI) (CA INDEX NAME)

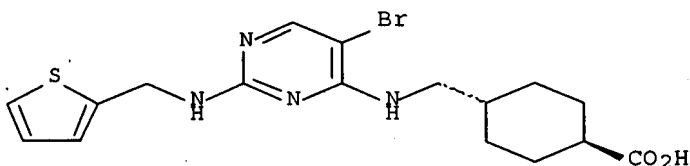
Absolute stereochemistry.



RN 557789-87-4 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[5-bromo-2-[(2-thienylmethyl)amino]-4-pyrimidinyl]amino]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 11 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:511301 CAPLUS Full-text

DOCUMENT NUMBER: 139:85041

TITLE: Heteroaryl-substituted aminocyclohexane derivatives as inhibitors of 2,3-oxidosqualene lanosterol cyclase

INVENTOR(S): Ackermann, Jean; Aebi, Johannes; Dehmlow, Henrietta; Maerki, Hans-Peter; Morand, Olivier

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: PCT Int. Appl., 83 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| WO 2003053933 | A1 | 20030703 | WO 2002-EP14037 | 20021211 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, | | | | |

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
 UG, UZ, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ,
 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003186984 A1 20031002 US 2002-310559 20021205 <--
 US 7012077 B2 20060314
 CA 2469380 A1 20030703 CA 2002-2469380 20021211 <--
 AU 2002366732 A1 20030709 AU 2002-366732 20021211 <--
 EP 1458683 A1 20040922 EP 2002-790481 20021211 <--
 EP 1458683 B1 20061122

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 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

BR 2002015257 A 20041207 BR 2002-15257 20021211 <--
 CN 1610669 A 20050427 CN 2002-825665 20021211 <--
 JP 2005517667 T 20050616 JP 2003-554649 20021211 <--
 RU 2286987 C2 20061110 RU 2004-122480 20021211 <--
 AT 346045 T 20061215 AT 2002-790481 20021211 <--

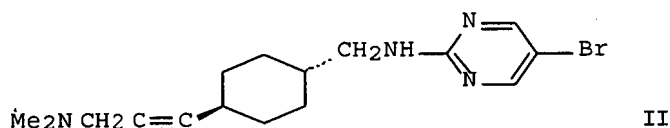
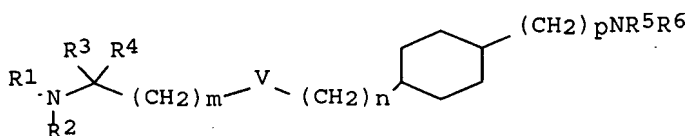
PRIORITY APPLN. INFO.:

EP 2001-130284 A 20011220 <--
 WO 2002-EP14037 W 20021211 <--

OTHER SOURCE(S): MARPAT 139:85041

ED Entered STN: 04 Jul 2003

GI



AB Title compds. I [R1 = H, alkyl, hydroxyalkyl, alkenyl; R2 = (un)substituted alkyl, cycloalkyl, cycloalkylalkyl, alkenyl; NR1R2 = heterocyclic; R3, R4 = H, alkyl; R3R4 = (CH2)5; R5 = H, alkyl, alkenyl; R6 = (un)substituted pyridinyl, pyridazinyl, pyrimidinyl, pyrazinyl; V = bond, O, S, CH:CHCH2O, CH:CH, C.tplbond.C; m, n = 0-7; p = 0-2] and their N-oxides were prepared for use as 2,3-oxidosqualene lanosterol cyclase inhibitors in treating diseases such as hypercholesterolemia, hyperlipemia, arteriosclerosis, vascular diseases, mycoses, parasitic infections, gallstones, tumors and/or hyperproliferative disorders, and treatment and/or prophylaxis of impaired glucose tolerance and diabetes. Thus, trans-3-{4-[(5-bromo-2-pyrimidinyl)methylaminocyclohexyl]prop-2-yn-1-ol, prepared from trans-4-tert.-butoxycarbonylaminocyclohexanecarboxylic acid and 2,5-dibromopyrimidine via trans-3-(4-methylaminocyclohexyl)prop-2-yn-1-ol, was converted to its mesylate and treated with Me2NH to give the title compound II.

IT 553677-39-7P 553677-40-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

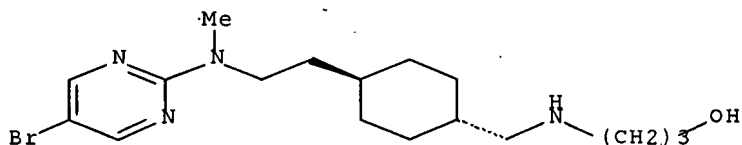
(Reactant or reagent)

(preparation of heteroaryl-substituted aminocyclohexane derivs. as inhibitors of 2,3-oxidosqualene lanosterol cyclase)

RN 553677-39-7 CAPLUS

CN 1-Propanol, 3-[[[trans-4-[2-[(5-bromo-2-pyrimidinyl)methylamino]ethyl]cyclohexyl]methyl]amino]- (9CI) (CA INDEX NAME)

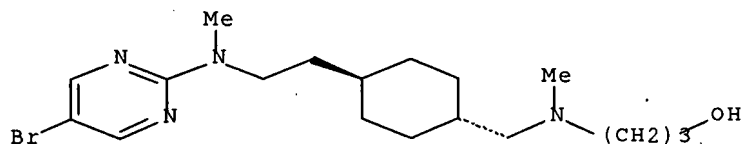
Relative stereochemistry.



RN 553677-40-0 CAPLUS

CN 1-Propanol, 3-[[[trans-4-[2-[(5-bromo-2-pyrimidinyl)methylamino]ethyl]cyclohexyl]methyl]methylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 553676-54-3P 553676-55-4P 553676-56-5P

553676-57-6P 553676-71-4P 553677-00-2P

553677-02-4P 553677-37-5P

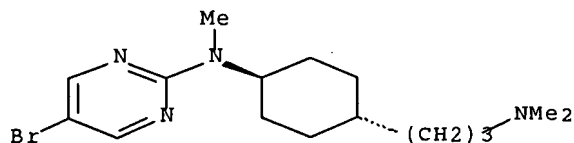
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heteroaryl-substituted aminocyclohexane derivs. as inhibitors of 2,3-oxidosqualene lanosterol cyclase)

RN 553676-54-3 CAPLUS

CN 2-Pyrimidinamine, 5-bromo-N-[trans-4-[3-(dimethylamino)propyl]cyclohexyl]-N-methyl- (9CI) (CA INDEX NAME)

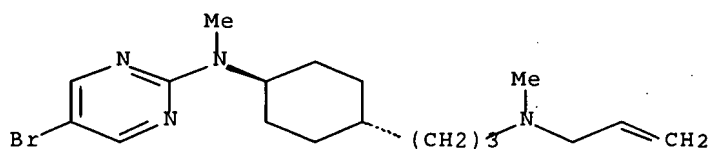
Relative stereochemistry.



RN 553676-55-4 CAPLUS

CN 2-Pyrimidinamine, 5-bromo-N-methyl-N-[trans-4-[3-(methyl-2-propenylamino)propyl]cyclohexyl]- (9CI) (CA INDEX NAME)

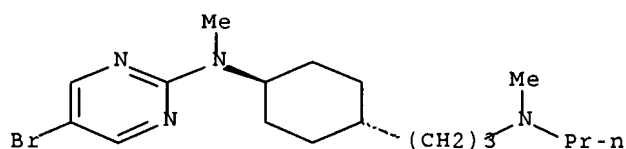
Relative stereochemistry.



RN 553676-56-5 CAPLUS

CN 2-Pyrimidinamine, 5-bromo-N-methyl-N-[trans-4-[3-(methylpropylamino)propyl]cyclohexyl]- (9CI) (CA INDEX NAME)

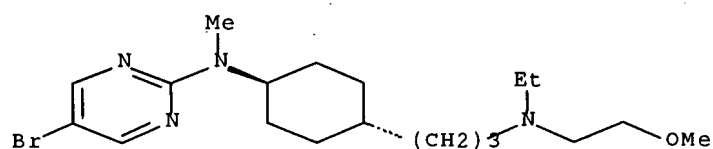
Relative stereochemistry.



RN 553676-57-6 CAPLUS

CN 2-Pyrimidinamine, 5-bromo-N-[trans-4-[3-[ethyl(2-methoxyethyl)amino]propyl]cyclohexyl]-N-methyl- (9CI) (CA INDEX NAME)

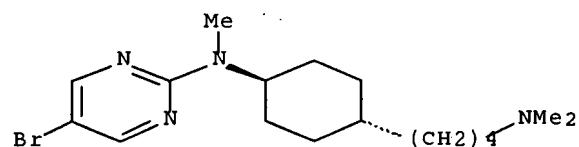
Relative stereochemistry.



RN 553676-71-4 CAPLUS

CN 2-Pyrimidinamine, 5-bromo-N-[trans-4-[4-(dimethylamino)butyl]cyclohexyl]-N-methyl- (9CI) (CA INDEX NAME)

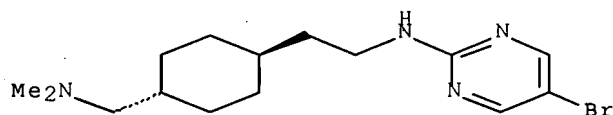
Relative stereochemistry.



RN 553677-00-2 CAPLUS

CN 2-Pyrimidinamine, 5-bromo-N-[2-[trans-4-[(dimethylamino)methyl]cyclohexyl]ethyl]- (9CI) (CA INDEX NAME)

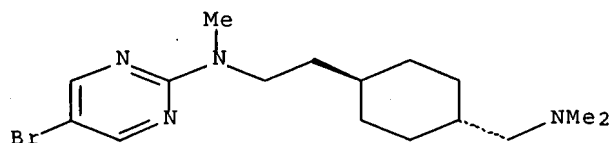
Relative stereochemistry.



RN 553677-02-4 CAPLUS

CN 2-Pyrimidinamine, 5-bromo-N-[2-[trans-4-[(dimethylamino)methyl]cyclohexyl]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

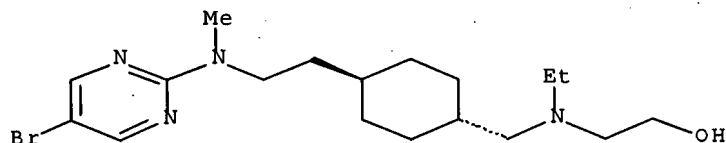
Relative stereochemistry.



RN 553677-37-5 CAPLUS

CN Ethanol, 2-[[[trans-4-[2-[(5-bromo-2-pyrimidinyl)methylamino]ethyl]cyclohexyl]methyl]ethylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 12 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:376852 CAPLUS Full-text

DOCUMENT NUMBER: 138:385443

TITLE: Preparation of amino imidazolyl pyrimidinecarboxaldehyde thiosemicarbazones, pyridine analogs and related compounds as inhibitors of IkB kinases

INVENTOR(S): Hawley, Ronald Charles; Labadie, Sharada Shenvi; Sjogren, Eric Brian; Talamas, Francisco Xavier

PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.

SOURCE: PCT Int. Appl., 98 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| WO 2003040131 | A1 | 20030515 | WO 2002-EP12164 | 20021031 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, | | | | |

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, UZ, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
 CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
 PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
 NE, SN, TD, TG

| | | | | |
|--|----|----------|-----------------|--------------|
| CA 2465711 | A1 | 20030515 | CA 2002-2465711 | 20021031 <-- |
| AU 2002350657 | A1 | 20030519 | AU 2002-350657 | 20021031 <-- |
| EP 1444223 | A1 | 20040811 | EP 2002-785344 | 20021031 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| BR 2002013899 | A | 20040831 | BR 2002-13899 | 20021031 <-- |
| CN 1582284 | A | 20050216 | CN 2002-822194 | 20021031 <-- |
| JP 2005511608 | T | 20050428 | JP 2003-542177 | 20021031 <-- |
| US 2003144303 | A1 | 20030731 | US 2002-288968 | 20021106 <-- |
| US 6846828 | B2 | 20050125 | | |
| US 2005107403 | A1 | 20050519 | US 2004-967430 | 20041018 <-- |
| US 7157580 | B2 | 20070102 | | |

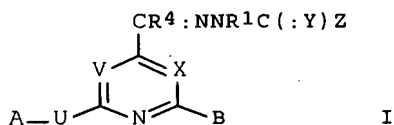
PRIORITY APPLN. INFO.:

| | | |
|-----------------|----|--------------|
| US 2001-338312P | P | 20011107 <-- |
| WO 2002-EP12164 | W | 20021031 <-- |
| US 2002-288968 | A3 | 20021106 <-- |

OTHER SOURCE(S): MARPAT 138:385443

ED Entered STN: 16 May 2003

GI



AB The present invention relates to aminopyrimidine and aminopyridine derivs. (shown as I; variables defined below; e.g. 2-butylamino-6-(1-methyl-1H-imidazol-5-yl)pyrimidine-4-carboxaldehyde 2-methylthiosemicarbazone (1)) and methods for their preparation. The compds. are useful as inhibitors of Ikb kinases and, therefore, may be used for the treatment of inflammatory, metabolic or malignant conditions (e.g. rheumatoid arthritis, inflammatory bowel disease, psoriasis, cancer, diabetes and septic shock). IC50 values for inhibition of IKK β enzyme activity are reported for 3 examples of I; e.g. 0.314 μ M for 1. Eleven example preps. of intermediates and I and characterization data for apprx.150 I are included. For example, 2-isopropylamino-6-(1-methyl-1H-imidazol-5-yl)pyrimidine-4-carboxaldehyde 2-methylthiosemicarbazone was prepared in 7 steps starting from Et diethoxyacetate, thiourea and benzyl bromide giving 2-benzylsulfanyl-6-diethoxymethylpyrimidin-4-ol as the 1st intermediate (50%); this intermediate was sequentially converted to the chloride (74%), pyrimidine imidazole, sulfone (31% for 2 steps), amino pyrimidine acetal (66%), aldehyde (64%) and finally the aldehyde thiosemicarbazone (71%). For I: one of either V or X is N and the other is CRa, or both V and X are CRa (Ra = H, (C1-C6)alkyl, (C3-C7)cycloalkyl or (C3-C7)cycloalkyl(C1-C6)alkyl); Y is O, S or NR (R is H, CN, NO2, (C1-C10)alkyl, (C3-C7)cycloalkyl, (C3-C7)cycloalkyl-(C1-C6)alkyl, (C3-C10)alkenyl or (C2-C10)alkynyl). Z is H, (C1-C6)alkyl, (C3-C7)cycloalkyl, (C3-C6)cycloalkyl(C1-C6)alkyl, (C2-C6)alkenyl, (C2-C6)alkynyl or N(R2)(R3); R1

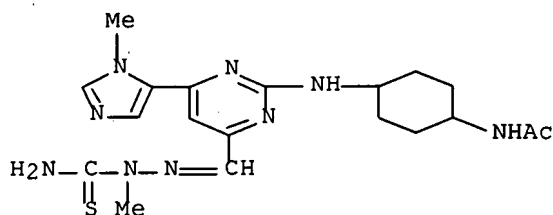
is H, (C1-C10)alkyl, (C3-C10)alkenyl, (C2-C10)alkynyl, (C3-C7)cycloalkyl, (C3-C7)cycloalkyl(C1-C6)alkyl, (C1-C10)heteroalkyl, heterocyclyl, heterocyclyl(C1-C6)alkyl, aryl, aryl(C1-C4)alkyl, aryl(C1-C4)heteroalkyl, heteroaryl(C1-C4)alkyl, heteroaryl(C1-C4)heteroalkyl, C(O)R11 or (C1-C6)alkylene-C(O)R11;. R4 is H, (C1-C6)alkyl, (C3-C7)cycloalkyl, (C3-C7)cycloalkyl(C1-C6)alkyl, (C2-C6)alkenyl or (C2-C6)alkynyl; A is H, (C1-C10)alkyl, (C3-C10)alkenyl, (C2-C10)alkynyl, halo (C1-C6)alkyl, (C3-C7)cycloalkyl, (C3-C7)cycloalkyl(C1-C6)alkyl, (C1-C10)heteroalkyl, heterocyclyl, heterocyclyl(C1-C6)alkyl, heterosubstituted (C3-C7)cycloalkyl, aryl, aryl(C1-C4)alkyl, aryl(C1-C4)heteroalkyl, heteroaryl, heteroaryl(C1-C4)alkyl, heteroaryl(C1-C4)heteroalkyl or RaRbNC(:X) (Ra and Rb = H, (C1-C4)alkyl or aryl). X is O or S; B is a (un)substituted five- or six-membered aromatic ring containing at least 1 N and 0-3 addnl. heteroatoms, wherein the B ring substituents = halogen, CF3, CF3O, (C1-C6)alkyl, amino, (C1-C6)alkylamino, di(C1-C6)alkylamino, cyano, nitro, sulfonamido, acyl, acylamino and carboxamido; U is -NR5-, -O- or -S-; addnl. details are given in the claims.

IT 525559-73-3P, 2-((4-(Acetylamino)cyclohexyl)amino)-6-(1-methyl-1H-imidazol-5-yl)pyrimidine-4-carboxaldehyde 2-methylthiosemicarbazone
525559-79-9P, 2-((4-((Methylsulfonyl)amino)cyclohexyl)amino)-6-(1-methyl-1H-imidazol-5-yl)pyrimidine-4-carboxaldehyde 2-methylthiosemicarbazone 525560-05-8P; 2-((3-((Methylsulfonyl)amino)cyclohexyl)amino)-6-(1-methyl-1H-imidazol-5-yl)pyrimidine-4-carboxaldehyde 2-methylthiosemicarbazone
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of amino imidazolyl pyrimidinecarboxaldehyde thiosemicarbazones, pyridine analogs and related compds. as inhibitors of Ikb kinases)

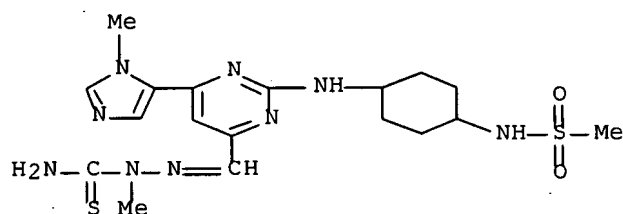
RN 525559-73-3 CAPLUS

CN Acetamide, N-[4-[[4-[[[(aminothioxomethyl)methylhydrazono]methyl]-6-(1-methyl-1H-imidazol-5-yl)-2-pyrimidinyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)



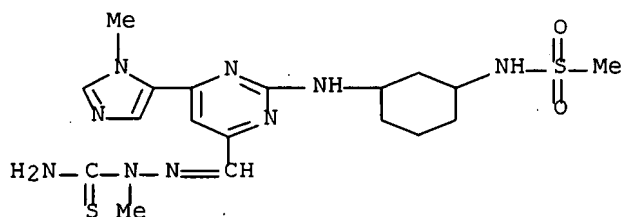
RN 525559-79-9 CAPLUS

CN Hydrazinecarbothioamide, 1-methyl-2-[[[6-(1-methyl-1H-imidazol-5-yl)-2-[[4-((methylsulfonyl)amino)cyclohexyl]amino]-4-pyrimidinyl]methylene]- (9CI) (CA INDEX NAME)



RN 525560-05-8 CAPLUS

CN Hydrazinecarbothioamide, 1-methyl-2-[[6-(1-methyl-1H-imidazol-5-yl)-2-[[3-[(methylsulfonyl)amino]cyclohexyl]amino]-4-pyrimidinyl]methylene]- (9CI)
(CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 13 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:335096 CAPLUS Full-text

DOCUMENT NUMBER: 138:353990

TITLE: Preparation of 4-imidazolin-2-one derivatives as MAP kinase inhibitors

INVENTOR(S): Kubo, Akira; Imashiro, Ritsuo; Sakurai, Hiroaki; Miyoshi, Hidetaka; Ogasawara, Akihito; Hiramatsu, Hajime

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 137 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| WO 2003035638 | A1 | 20030501 | WO 2002-JP10937 | 20021022 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2461100 | A1 | 20030501 | CA 2002-2461100 | 20021022 <-- |
| AU 2002363108 | A1 | 20030506 | AU 2002-363108 | 20021022 <-- |
| EP 1439174 | A1 | 20040721 | EP 2002-802049 | 20021022 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| BR 2002013465 | A | 20041109 | BR 2002-13465 | 20021022 <-- |
| CN 1571781 | A | 20050126 | CN 2002-820837 | 20021022 <-- |
| HU 200401949 | A2 | 20050128 | HU 2004-1949 | 20021022 <-- |
| US 2004204426 | A1 | 20041014 | US 2004-827294 | 20040420 <-- |

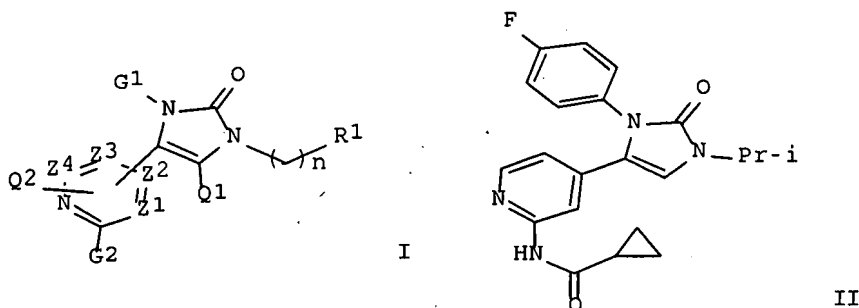
NO 2004002010
PRIORITY APPLN. INFO.:

A 20040709

NO 2004-2010
JP 2001-324029
JP 2002-263680
WO 2002-JP10937
JP 2003-116076

20040514 <--
A 20011022 <--
A 20020910 <--
W 20021022 <--
A 20030421

OTHER SOURCE(S): MARPAT 138:353990
ED Entered STN: 02 May 2003
GI



AB The title compds. I [wherein G1 = (un)substituted alkyl or B-W; B = (un)substituted Ph, Naphthyl, aromatic heterocyclyl, or cycloalkyl; W = a single bond or (un)substituted alkylene; Q1 and Q2 = independently H, halo, or alkyl; n = 0-4; R1 = H, (un)substituted (cyclo)alkyl, Ph, or heterocyclyl; Z1-Z4 = independently CH or N with exclusions; G2 = H, NR3R4, OR5, SR5, COR6, CHR7R8, or heterocyclyl; R3-R8 = independently H, alkenyl, alkynyl, OH, alkoxy, alkoxyoxalyl, alkylsulfonyl, (un)substituted alkyl, amino, alkanoyl, carbamoyl, cycloalkyl, Ph, heterocyclyl(carbonyl), PhCO, or heterocyclyl-CO] and pharmaceutically acceptable salts are prepared as mitogen activation proteins (MAP) kinase inhibitors. For example, the compound II•HCl was prepared in a multi-step synthesis. II•HCl showed 69% inhibitory activity against TNF- α in rat in the amount of 1 mg/kg after 90 min.

IT 521090-75-5P 521090-76-6P 521091-56-5P
521091-59-8P 521091-62-3P 521091-63-4P
521091-65-6P

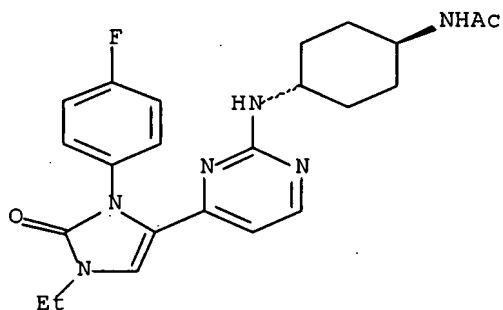
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(MAP kinase inhibitor; preparation of imidazolinone derivs. as MAP kinase inhibitors)

RN 521090-75-5 CAPLUS

CN Acetamide, N-[trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI)
(CA INDEX NAME)

Relative stereochemistry.

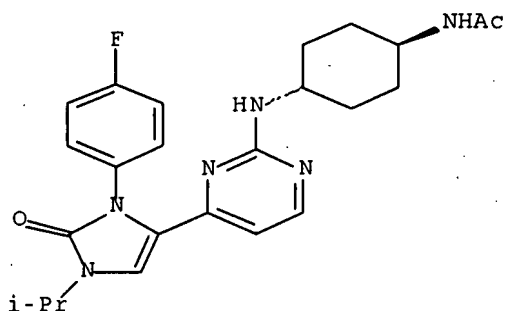


● HCl

RN 521090-76-6 CAPLUS

CN Acetamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

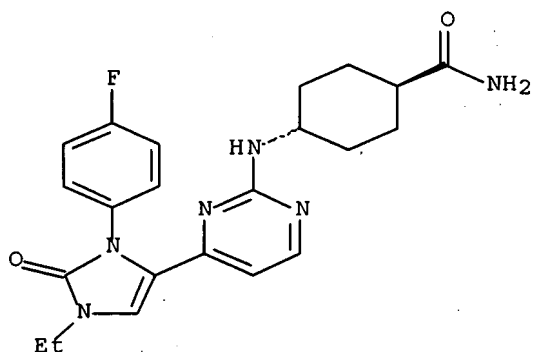


● HCl

RN 521091-56-5 CAPLUS

CN Cyclohexanecarboxamide, 4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

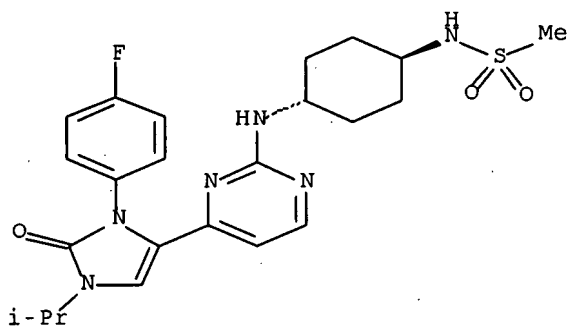


● HCl

RN 521091-59-8 CAPLUS

CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

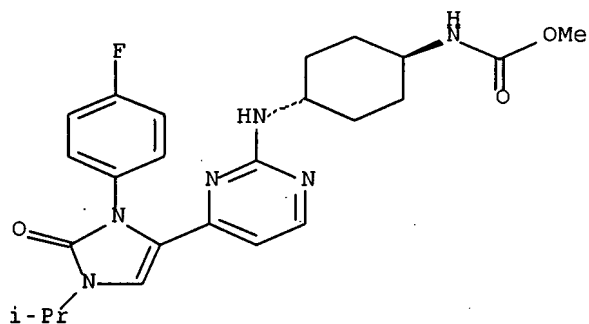


● HCl

RN 521091-62-3 CAPLUS

CN Carbamic acid, [trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

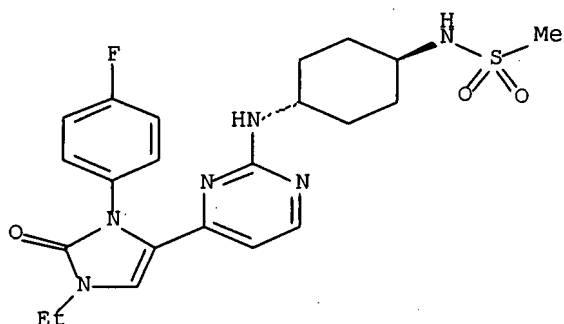


● HCl

RN 521091-63-4 CAPLUS

CN Methanesulfonamide, N-[trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

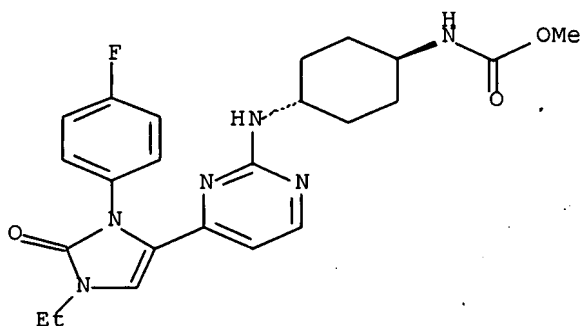


● HCl

RN 521091-65-6 CAPLUS

CN Carbamic acid, [trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

REFERENCE COUNT: 99 THERE ARE 99 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 14 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:319721 CAPLUS Full-text

DOCUMENT NUMBER: 138:321292

TITLE: Preparation of 2,4,5-trisubstituted pyrimidines as cyclin dependent kinase inhibitors

INVENTOR(S): Dahmann, Georg; Himmelsbach, Frank; Wittneben, Helmut; Pautsch, Alexander; Prokopowicz, Anthony S.; Krist, Bernd; Schnapp, Gisela; Steegmaier, Martin; Lenter, Martin; Schoop, Andreas; Steurer, Steffen; Spevak, Walter

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany; Boehringer Ingelheim Pharmaceuticals, Inc.; Boehringer Ingelheim International G.m.b.H.

SOURCE: PCT Int. Appl., 278 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

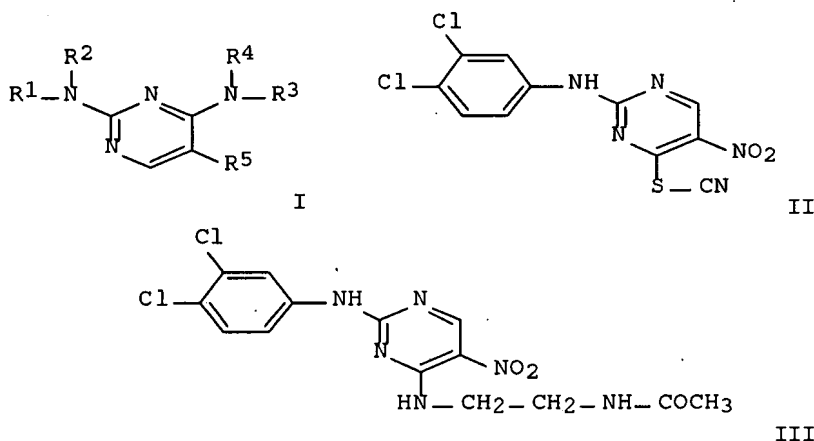
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| WO 2003032997 | A1 | 20030424 | WO 2002-EP11453 | 20021014 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2463989 | A1 | 20030424 | CA 2002-2463989 | 20021014 <-- |
| AU 2002340560 | A1 | 20030428 | AU 2002-340560 | 20021014 <-- |
| EP 1438053 | A1 | 20040721 | EP 2002-774710 | 20021014 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| JP 2005509624 | T | 20050414 | JP 2003-535800 | 20021014 <-- |
| US 2003171359 | A1 | 20030911 | US 2002-271763 | 20021016 <-- |

US 7173028 B2 20070206
 US 2006100211 A1 20060511 US 2005-313380 20051221 <--
 PRIORITY APPLN. INFO.: US 2001-330145P P 20011017 <--
 WO 2002-EP11453 W 20021014 <--
 US 2002-271763 A3 20021016 <--

OTHER SOURCE(S): MARPAT 138:321292
 ED Entered STN: 25 Apr 2003
 GI



AB Title compds. I [R1 = H, alkyl; R2 = (un)substituted alkyl; R3 = H, alkyl; R4 = (un)substituted alkyl; R5 = halo] and their pharmaceutically acceptable salts were prepared. For example, condensation of thiocyanatopyrimidine II, e.g., prepared from 3,4-dichloroaniline and 2-chloro-4-thiocyanato-5-nitropyrimidine in one step, and acetylaminoethylamine provided trisubstituted pyrimidine III in 88% yield. In CDK1/CyclinB1 kinase inhibition studies, 88-examples of compds. I exhibited IC50 values more than 100 nM. Compds. I are claimed useful for the treatment of diseases characterized by abnormal cell proliferation.

IT 514830-77-4P, 2-(4-Carboxyphenylamino)-4-((trans-4-(dimethylamino)cyclohexyl)amino)-5-nitropyrimidine 514831-13-1P, 2-(4-Carboxyphenylamino)-4-(trans-4-dimethylaminocyclohexylamino)-5-trifluoromethylpyrimidine 514831-20-0P, 2-(3,4-Dichlorophenylamino)-4-(trans-4-carboxycyclohexylamino)-5-trifluoromethylpyrimidine 514831-41-5P, 2-(3,4-Dichlorophenylamino)-4-(((4-(N,N-dimethylaminomethyl)cyclohexyl)methyl)amino)-5-trifluoromethylpyrimidine 514831-79-9P, 2-(3,4-Dichlorophenylamino)-4-(4-dimethylaminocyclohexylamino)-5-trifluoromethylpyrimidine 514832-17-8P, 2-(3,4-Dichlorophenylamino)-4-[(4-(2-carboxyethyl)cyclohexyl)amino]-5-trifluoromethylpyrimidine 514832-18-9P, 2-(4-Chlorophenylamino)-4-((trans-4-carboxycyclohexyl)amino)-5-nitropyrimidine 514832-54-3P, 2-(3,4-Dichlorophenylamino)-4-(3-carboxycyclohexylamino)-5-trifluoromethylpyrimidine 514832-61-2P, 2-(4-Chlorophenylamino)-4-(4-dimethylaminocyclohexylamino)-5-nitropyrimidine 514832-72-5P, 2-(4-Chlorophenylamino)-4-(3-carboxycyclohexylamino)-5-nitropyrimidine 514832-73-6P, 2-(4-Chlorophenylamino)-4-[(4-(2-carboxyethyl)cyclohexyl)amino]-5-nitropyrimidine 514832-78-1P, 2-(4-Chlorophenylamino)-4-(((4-

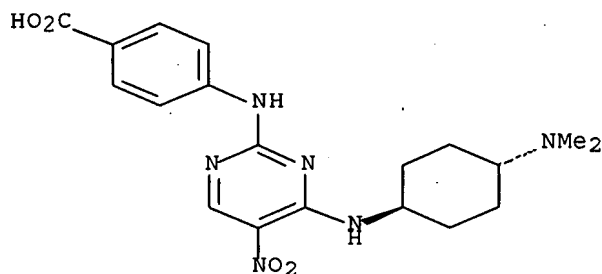
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 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of trisubstituted pyrimidines as cyclin dependent kinase inhibitors)

RN 514830-77-4 CAPLUS

CN Benzoic acid, 4-[[4-[[trans-4-(dimethylamino)cyclohexyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

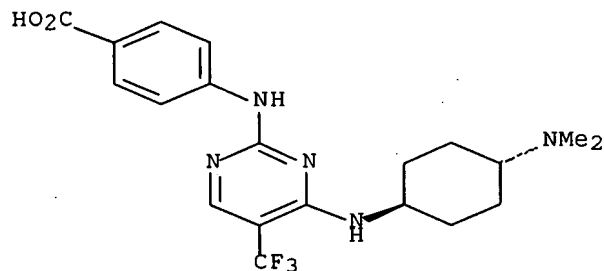
Relative stereochemistry.



RN 514831-13-1 CAPLUS

CN Benzoic acid, 4-[[4-[[trans-4-(dimethylamino)cyclohexyl]amino]-5-(trifluoromethyl)-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

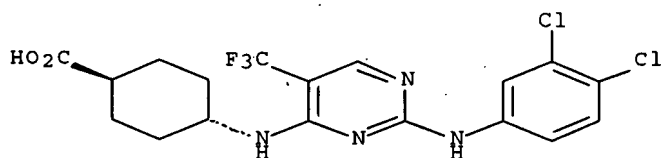
Relative stereochemistry.



RN 514831-20-0 CAPLUS

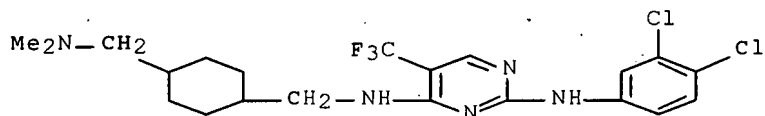
CN Cyclohexanecarboxylic acid, 4-[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



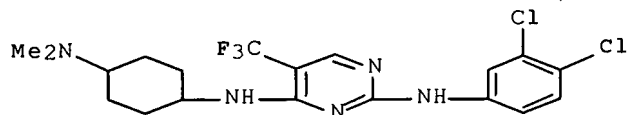
RN 514831-41-5 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[[4-[(dimethylamino)methyl]cyclohexyl]methyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



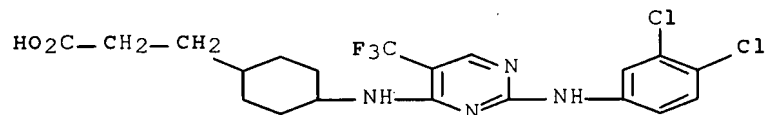
RN 514831-79-9 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[4-(dimethylamino)cyclohexyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 514832-17-8 CAPLUS

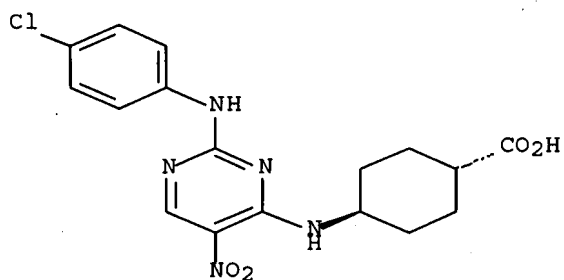
CN Cyclohexanepropanoic acid, 4-[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 514832-18-9 CAPLUS

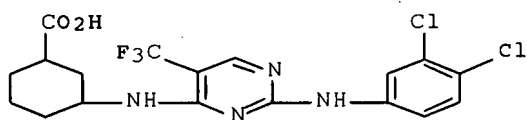
CN Cyclohexanecarboxylic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



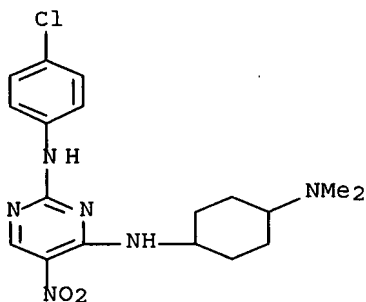
RN 514832-54-3 CAPLUS

CN 'Cyclohexanecarboxylic acid, 3-[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



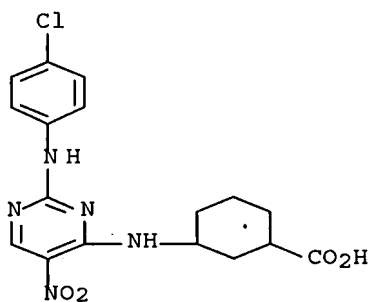
RN 514832-61-2 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[4-(dimethylamino)cyclohexyl]-5-nitro- (9CI) (CA INDEX NAME)



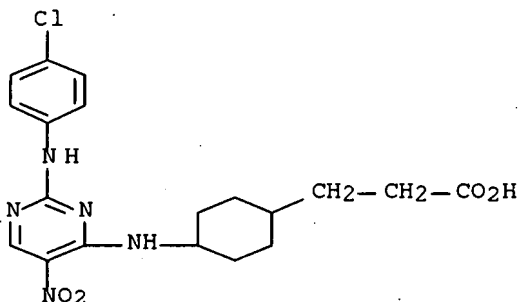
RN 514832-72-5 CAPLUS

CN Cyclohexanecarboxylic acid, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



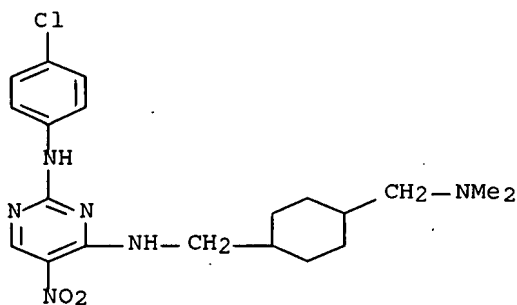
RN 514832-73-6 CAPLUS

CN Cyclohexanepropanoic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



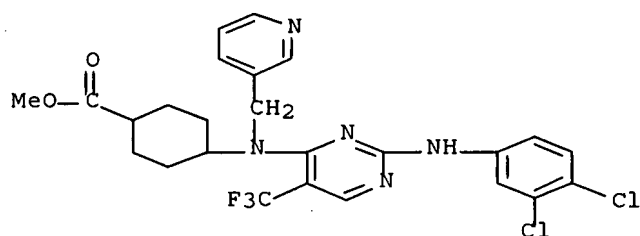
RN 514832-78-1 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[[4-[(dimethylamino)methyl]cyclohexyl]methyl]-5-nitro- (9CI) (CA INDEX NAME)



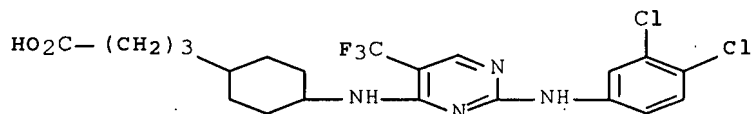
RN 514833-45-5 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]- (3-pyridinylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



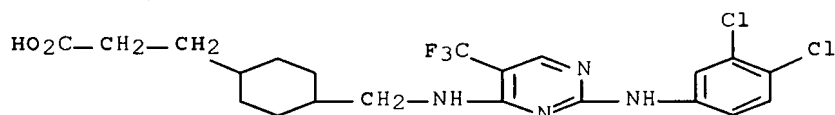
RN 514834-33-4 CAPLUS

CN Cyclohexanebutanoic acid, 4-[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



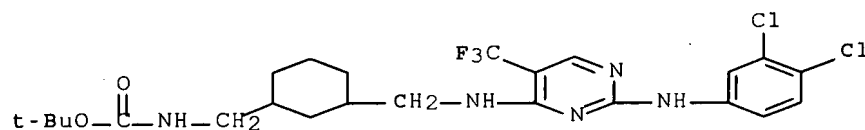
RN 514834-34-5 CAPLUS

CN Cyclohexanepropanoic acid, 4-[[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



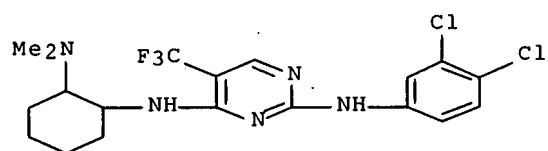
RN 514834-50-5 CAPLUS

CN Carbamic acid, [[3-[[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 514834-57-2 CAPLUS

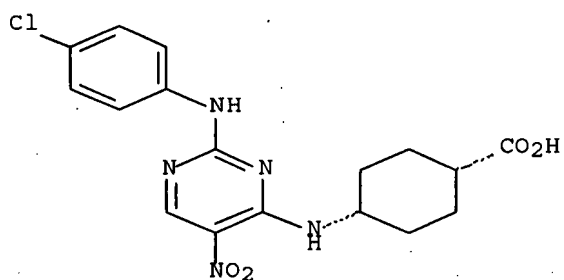
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[2-(dimethylamino)cyclohexyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 514835-37-1 CAPLUS .

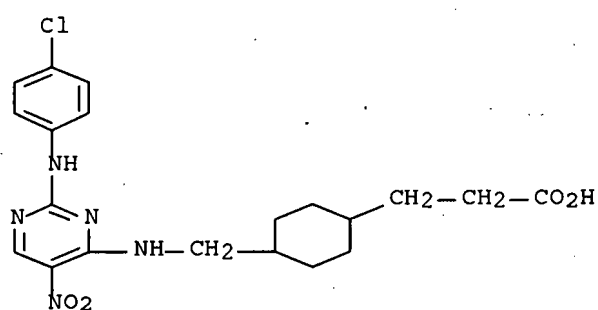
CN Cyclohexanecarboxylic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



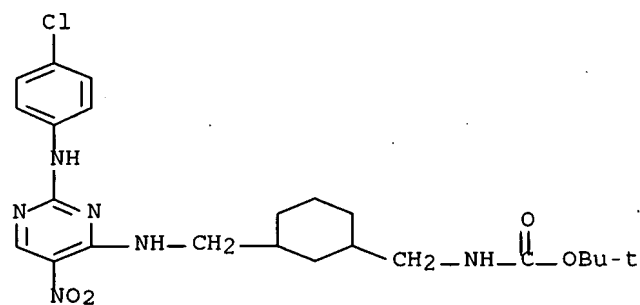
RN 514836-32-9 CAPLUS

CN Cyclohexanepropanoic acid, 4-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



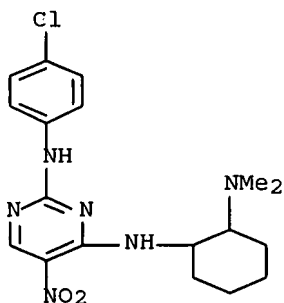
RN 514836-51-2 CAPLUS

CN Carbamic acid, [[3-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 514836-62-5 CAPLUS

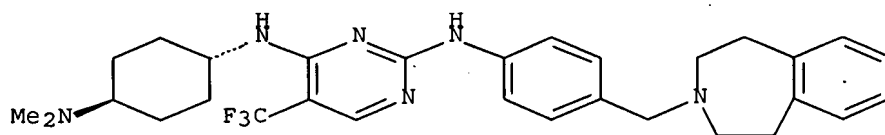
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(dimethylamino)cyclohexyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514837-09-3 CAPLUS

CN 2,4-Pyrimidinediamine, N4-[trans-4-(dimethylamino)cyclohexyl]-N2-[4-[(1,2,4,5-tetrahydro-3H-3-benzazepin-3-yl)methyl]phenyl]-5-(trifluoromethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

• Relative stereochemistry.



●2 HCl

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 15 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:927413 CAPLUS Full-text

DOCUMENT NUMBER: 138:14070

TITLE: CDK inhibiting pyrimidines

INVENTOR(S): Brumby, Thomas; Jautelat, Rolf; Prien, Olaf; Schaefer, Martina; Siemeister, Gerhard; Luecking, Ulrich; Huwe, Christoph

PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 240 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|--|----------|-----------------|--------------|
| WO 2002096888 | A1 | 20021205 | WO 2002-EP5669 | 20020523 <-- |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, | | | |

BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

| | | | | |
|---------------|----|----------|------------------|--------------|
| DE 10127581 | A1 | 20030102 | DE 2001-10127581 | 20010529 <-- |
| DE 10212098 | A1 | 20031023 | DE 2002-10212098 | 20020311 <-- |
| CA 2449118 | A1 | 20021205 | CA 2002-2449118 | 20020523 <-- |
| AU 2002312933 | A1 | 20021209 | AU 2002-312933 | 20020523 <-- |
| EP 1392662 | A1 | 20040303 | EP 2002-738100 | 20020523 <-- |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

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|----------------|----|----------|----------------|--------------|
| BR 2002009774 | A | 20040601 | BR 2002-9774 | 20020523 <-- |
| JP 2004535414 | T | 20041125 | JP 2003-500067 | 20020523 <-- |
| CN 1633419 | A | 20050629 | CN 2002-814886 | 20020523 <-- |
| NZ 529654 | A | 20051223 | NZ 2002-529654 | 20020523 <-- |
| US 2004102630 | A1 | 20040527 | US 2002-156759 | 20020529 <-- |
| US 7235561 | B2 | 20070626 | | |
| IN 2003DN02240 | A | 20060120 | IN 2003-DN2240 | 20031222 <-- |
| US 2004224966 | A1 | 20041111 | US 2004-842419 | 20040511 <-- |
| ZA 200309824 | A | 20060531 | ZA 2003-9824 | 20060320 <-- |

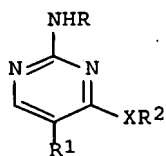
PRIORITY APPLN. INFO.:

| | | |
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| DE 2001-10127581 | A | 20010529 <-- |
| DE 2002-10212098 | A | 20020311 <-- |
| WO 2002-EP5669 | W | 20020523 <-- |
| US 2002-156759 | A3 | 20020529 <-- |

OTHER SOURCE(S): MARPAT 138:14070

ED Entered STN: 06 Dec 2002

GI



I

AB Pyrimidines I [R = (un)substituted Ph; R1 = H, halogen, (un)substituted alkyl, NO2, acyl, OCF3, SCF3, SO2CF3; R2 = (un)substituted alkyl, alkenyl, alkynyl; X = O, (un)substituted NH, cycloalkoxy; XR2 = (un)substituted cycloalkyl, heterocyclic] were prepared as inhibitors of the cyclin-dependent kinase. Thus, 2-chloro-4-propargylaminopyrimidine was treated with 4-F2CHSC6H4NH2.HCl to give I [X = NH, R = 4-F2CHSC6H4, R1 = Br, R2 = CH2C.tplbond.CH] which had IC50 for inhibition of CDK2 of 180 nM and for inhibition of MCF7 tumor cell proliferation of 3 μ M.

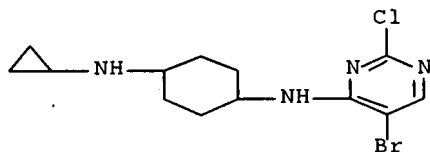
IT 477593-38-7P 477593-41-2P 477593-42-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclin-dependent kinase inhibition of arylaminopyrimidines)

RN 477593-38-7 CAPLUS

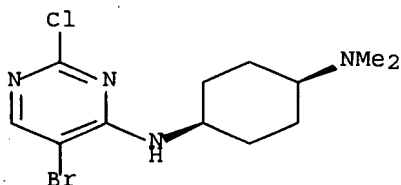
CN 1,4-Cyclohexanediamine, N-(5-bromo-2-chloro-4-pyrimidinyl)-N'-cyclopropyl- (9CI) (CA INDEX NAME)



RN 477593-41-2 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-bromo-2-chloro-4-pyrimidinyl)-N,N-dimethyl-,
cis- (9CI) (CA INDEX NAME)

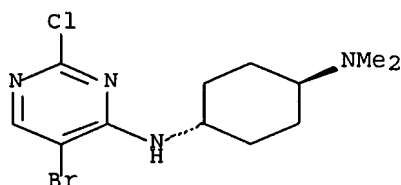
Relative stereochemistry.



RN 477593-42-3 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-bromo-2-chloro-4-pyrimidinyl)-N,N-dimethyl-,
trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 477589-08-5P 477589-09-6P 477589-12-1P

477589-16-5P 477589-17-6P 477589-48-3P

477589-49-4P 477589-51-8P 477589-52-9P

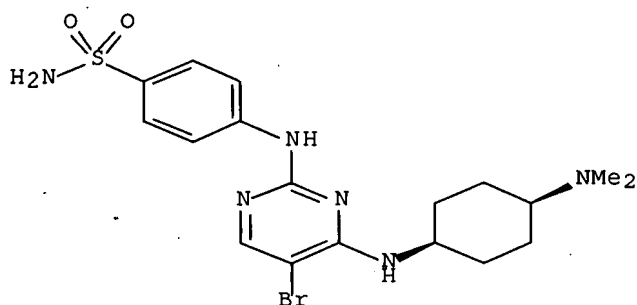
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and cyclin-dependent kinase inhibition of arylaminopyrimidines)

RN 477589-08-5 CAPLUS

CN Benzenesulfonamide, 4-[[[5-bromo-4-[[[cis-4-(dimethylamino)cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

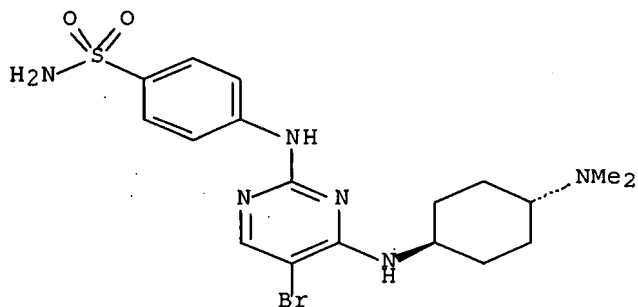
Relative stereochemistry.



RN 477589-09-6 CAPLUS

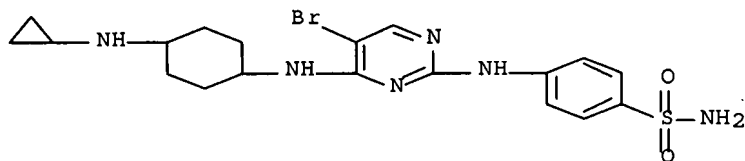
CN Benzenesulfonamide, 4-[[5-bromo-4-[[trans-4-(dimethylamino)cyclohexyl]amino]o]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



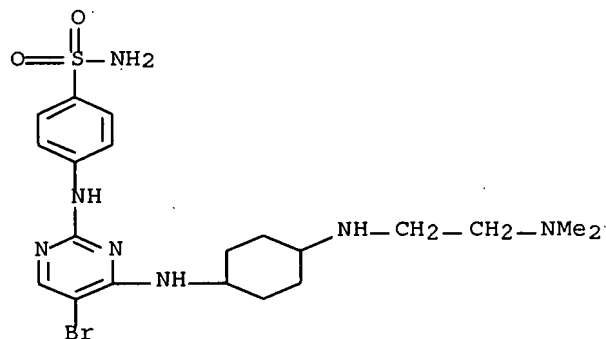
RN 477589-12-1 CAPLUS

CN Benzenesulfonamide, 4-[[5-bromo-4-[[4-(cyclopropylamino)cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



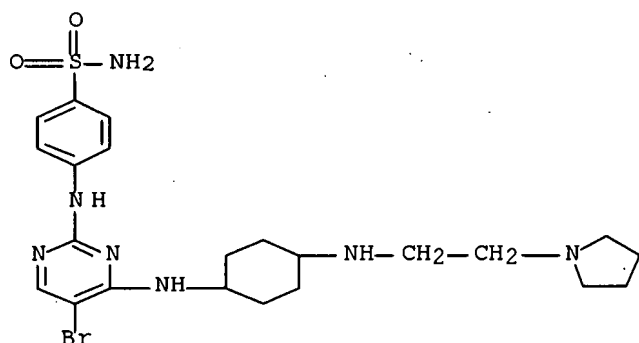
RN 477589-16-5 CAPLUS

CN Benzenesulfonamide, 4-[[5-bromo-4-[[4-[[2-(dimethylamino)ethyl]amino]cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 477589-17-6 CAPLUS

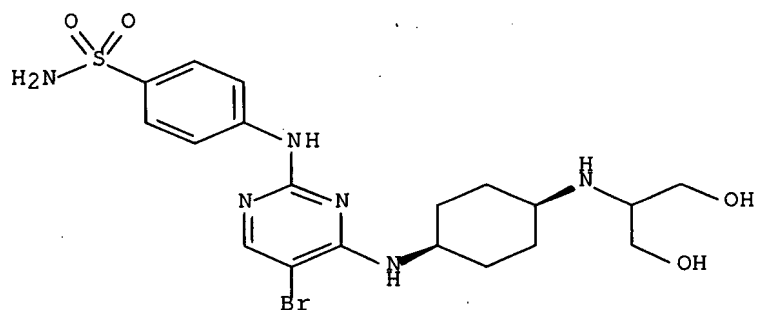
CN Benzenesulfonamide, 4-[[5-bromo-4-[[4-[[2-(1-pyrrolidinyl)ethyl]amino]cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 477589-48-3 CAPLUS

CN Benzenesulfonamide, 4-[[5-bromo-4-[[cis-4-[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]cyclohexyl]amino]-2-pyrimidinyl]amino] - (9CI)
(CA INDEX NAME)

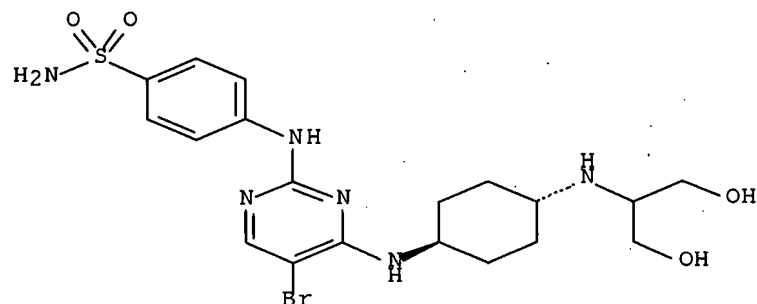
Relative stereochemistry.



RN 477589-49-4 CAPLUS

CN Benzenesulfonamide, 4-[[5-bromo-4-[[trans-4-[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]cyclohexyl]amino]-2-pyrimidinyl]amino] - (9CI)
(CA INDEX NAME)

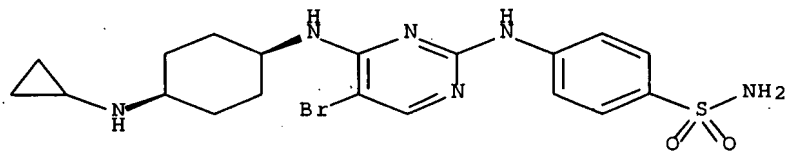
Relative stereochemistry.



RN 477589-51-8 CAPLUS

CN Benzenesulfonamide, 4-[[5-bromo-4-[[cis-4-(cyclopropylamino)cyclohexyl]amino]-2-pyrimidinyl]amino] - (9CI) (CA INDEX NAME)

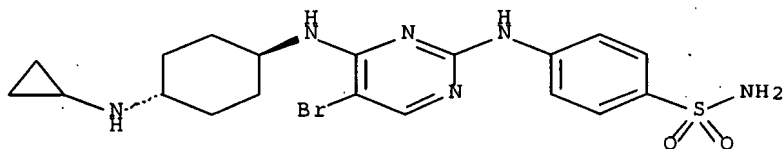
Relative stereochemistry.



RN 477589-52-9 CAPLUS

CN Benzenesulfonamide, 4-[[[5-bromo-4-[[trans-4-(cyclopropylamino)cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 16 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:878755 CAPLUS Full-text

DOCUMENT NUMBER: 139:17096

TITLE: Characterization of mono- and diaminopyrimidine derivatives as novel, nonpeptide gonadotropin releasing hormone (GnRH) receptor antagonists

AUTHOR(S): Luthin, David R.; Hong, Yufeng; Tompkins, Eileen; Anderes, Kenna L.; Paderes, Genevieve; Kraynov, Eugenia A.; Castro, Mary A.; Nared-Hood, Karen D.; Castillo, Rosemary; Gregory, Margaret; Vazir, Hareesh; May, John M.; Anderson, Mark B.

CORPORATE SOURCE: Pfizer Global Research and Development-La Jolla/Agouron Pharmaceuticals, Inc., 10724 Science Center Drive, San Diego, CA, 92121, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(24), 3635-3639

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:17096

ED Entered STN: 20 Nov 2002

AB A novel series of derivs. of mono- and diaminopyrimidines 1 potently displaced binding of a radiolabeled GnRH analog to human and rat GnRH receptors. Analogs from these series competitively antagonized GnRH-stimulated increases in extracellular acidification in vitro and suppressed GnRH-mediated increases in circulating LH (LH) in castrated rats and testosterone in intact rats. These compds. or their analogs may be useful in treating sex hormone-dependent disease.

IT 263848-23-3P 263848-26-6P 263848-44-8P
263848-45-9P 263848-46-0P 263848-62-0P
263848-88-0P 263849-24-7P 263849-27-0P

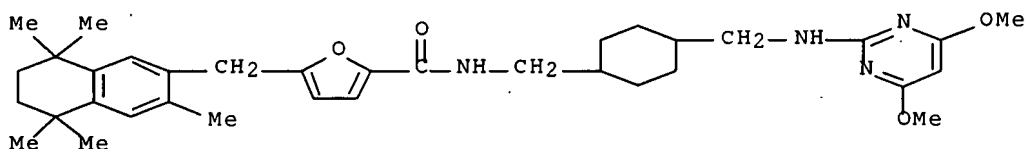
537696-28-9P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(characterization of mono- and diaminopyrimidine derivs. as novel, nonpeptide gonadotropin releasing hormone (GnRH) receptor antagonists)

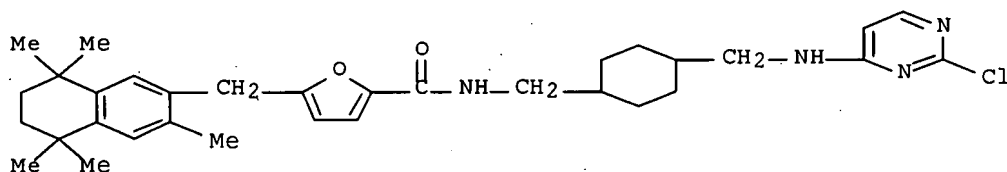
RN 263848-23-3 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[(4,6-dimethoxy-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]]- (9CI) (CA INDEX NAME)



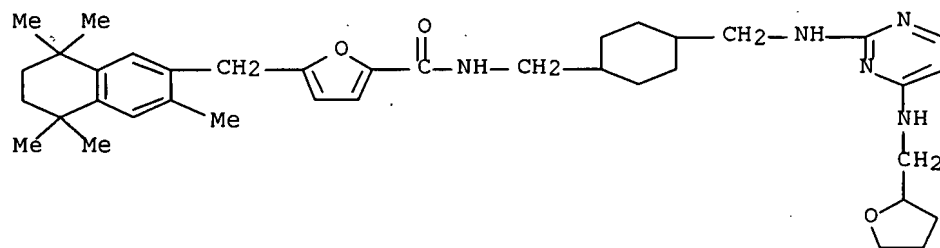
RN 263848-26-6 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[(2-chloro-4-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]]- (9CI) (CA INDEX NAME)



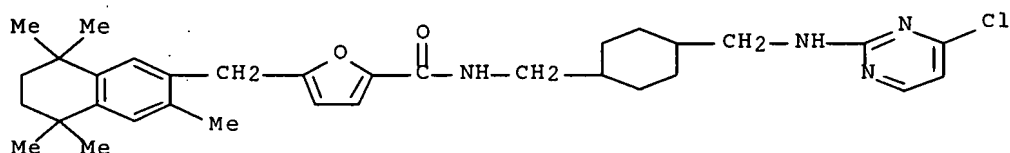
RN 263848-44-8 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[4-[[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]]- (9CI) (CA INDEX NAME)



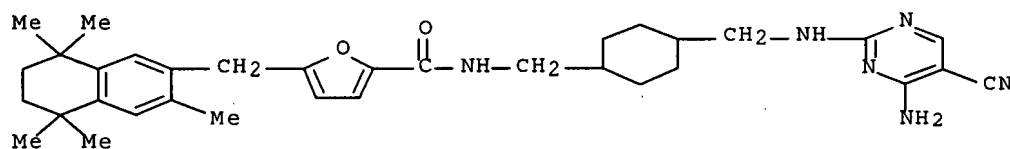
RN 263848-45-9 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[(4-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]]- (9CI) (CA INDEX NAME)



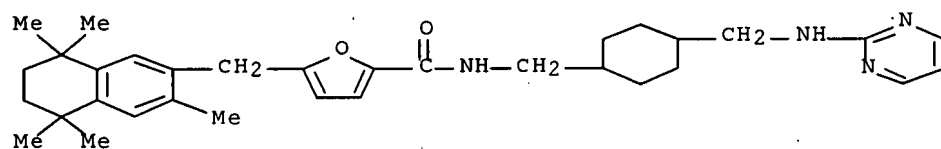
RN 263848-46-0 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[(4-amino-5-cyano-2-pyrimidinyl)amino)methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME)



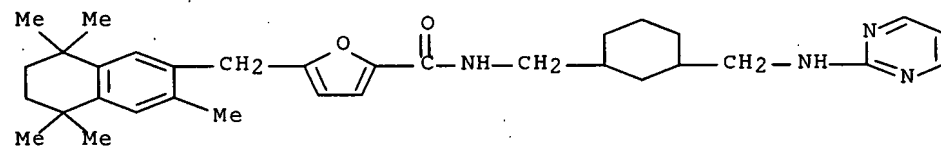
RN 263848-62-0 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[(2-pyrimidinylamino)methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME)



RN 263848-88-0 CAPLUS

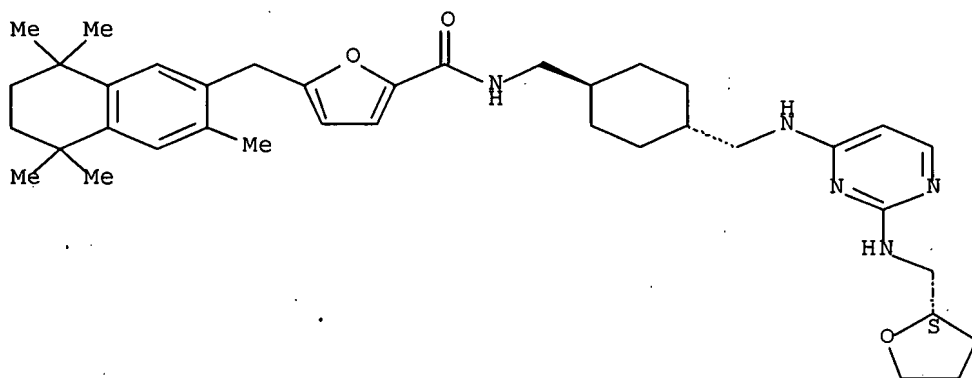
CN 2-Furancarboxamide, N-[[3-[[[(2-pyrimidinylamino)methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME)



RN 263849-24-7 CAPLUS

CN 2-Furancarboxamide, N-[[trans-4-[[[2-[[[(2S)-tetrahydro-2-furanyl]methyl]amino]-4-pyrimidinyl]amino)methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME)

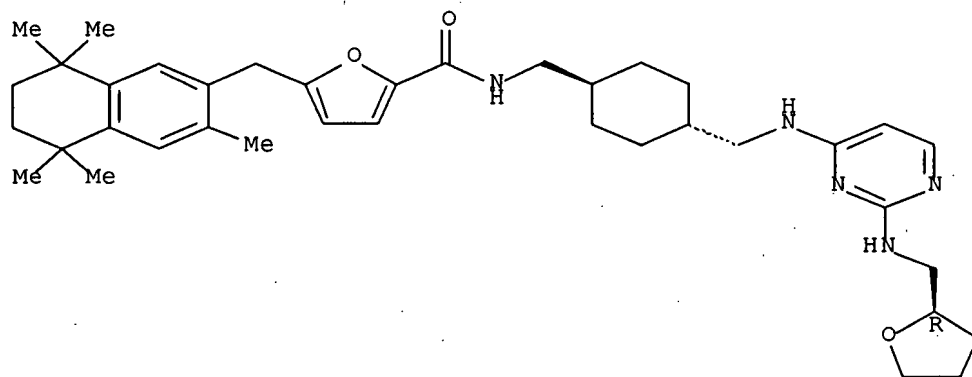
Absolute stereochemistry.



RN 263849-27-0 CAPLUS

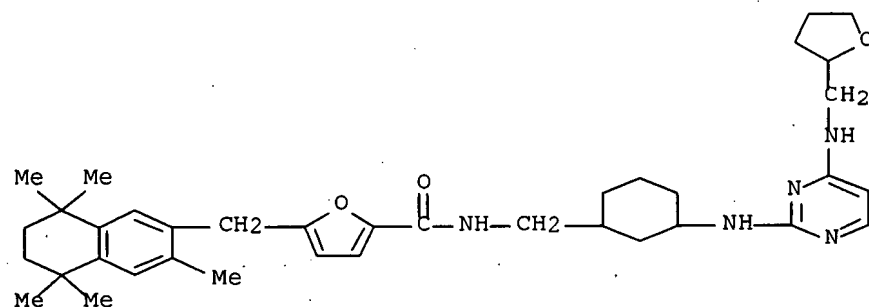
CN 2-Furancarboxamide, N-[[[trans-4-[[[2-[[[(2R)-tetrahydro-2-furanyl)methyl]amino]-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



RN 537696-28-9 CAPLUS

CN 2-Furancarboxamide, N-[[[3-[[4-[[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

18

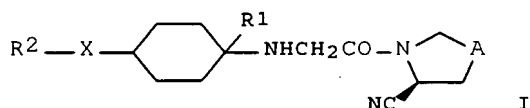
THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 17 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:293616 CAPLUS Full-text
 DOCUMENT NUMBER: 136:325560
 TITLE: Preparation of aliphatic nitrogenous five-membered
 ring compounds as dipeptidyl peptidase IV inhibitors
 INVENTOR(S): Yasuda, Kosuke; Morimoto, Hiroshi; Kawanami, Saburo;
 Hikota, Masataka; Matsumoto, Takeshi; Arakawa, Kenji
 PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 164 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|-----------------|
| WO 2002030891 | A1 | 20020418 | WO 2001-JP8803 | 20011005 <-- |
| W: AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CO, CR, CU, CZ, DM, DZ, EC, EE, GD, GE, HR, HU, ID, IL, IN, IS, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PH, PL, RO, SG, SI, SK, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 200194197 | A | 20020422 | AU 2001-94197 | 20011005 <-- |
| JP 2002356471 | A | 20021213 | JP 2001-309558 | 20011005 <-- |
| JP 2002356472 | A | 20021213 | JP 2001-309559 | 20011005 <-- |
| CA 2424600 | A1 | 20030402 | CA 2001-2424600 | 20011005 <-- |
| BR 2001014436 | A | 20030701 | BR 2001-14436 | 20011005 <-- |
| EP 1325910 | A1 | 20030709 | EP 2001-974717 | 20011005 <-- |
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| CN 1468216 | A | 20040114 | CN 2001-816674 | 20011005 <-- |
| HU 200303391 | A2 | 20040301 | HU 2003-3391 | 20011005 <-- |
| NZ 524974 | A | 20051028 | NZ 2001-524974 | 20011005 <-- |
| CN 1891689 | A | 20070110 | CN 2006-10077863 | 20011005 <-- |
| IN 2003KN00303 | A | 20050311 | IN 2003-KN303 | 20030312 <-- |
| ZA 2003002030 | A | 20030926 | ZA 2003-2030 | 20030313 <-- |
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| US 2004063935 | A1 | 20040401 | US 2003-398486 | 20030404 <-- |
| US 6849622 | B2 | 20050201 | | |
| JP 2004035574 | A | 20040205 | JP 2003-368572 | 20031029 <-- |
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| US 7160877 | B2 | 20070109 | | |
| AU 2004237882 | A1 | 20050106 | AU 2004-237882 | 20041213 <-- |
| JP 2005200427 | A | 20050728 | JP 2005-105732 | 20050401 <-- |
| PRIORITY APPLN. INFO.: | | | | |
| | | | JP 2000-308528 | A 20001006 <-- |
| | | | JP 2000-312562 | A 20001012 <-- |
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| | | | CN 2001-816674 | A3 20011005 <-- |
| | | | JP 2001-309558 | A3 20011005 <-- |
| | | | JP 2001-309559 | A3 20011005 <-- |
| | | | WO 2001-JP8803 | W 20011005 <-- |
| | | | US 2003-398486 | A3 20030404 |

OTHER SOURCE(S): MARPAT 136:325560
 ED Entered STN: 19 Apr 2002
 GI



AB Aliphatic nitrogenous five-membered ring compds., (S)-N-(N-cyclohexylglycyl)pyrrolidine-2-carbonitrile and (R)-N-(N-cyclohexylglycyl)thiazolidine-2-carbonitrile, of the general formula (I) or pharmacol. acceptable salts thereof [wherein A is CH₂ or S; R₁ is hydrogen, lower alkyl, hydroxy-lower alkyl, or lower alkoxy-lower alkyl; X is N(R₃), O, or CO; R₃ is hydrogen or lower alkyl; and R₂ is an optionally substituted mono- or bicyclic hydrocarbyl or heterocyclyl group or optionally substituted amino] are prepared. These compds. are useful as dipeptidyl peptidase IV inhibitors for the prevention or treatment of diabetes, in particular type II diabetes (no data). Thus, a solution of (S)-1-bromoacetyl-2-cyanopyrrolidine and N-(5-nitro-2-pyridyl)-trans-1,4-cyclohexanediamine in MeOH/MeCN was stirred at room temperature for 15 h to give, after treatment with 2 N HCl/Et₂O in EtOAc/CHCl₃, (S)-2-cyano-1-[[[trans-4-(5-nitro-2-pyridylamino)cyclohexyl]amino]acetyl]pyrrolidine dihydrochloride.

IT 412284-89-0P 412284-90-3P 412284-91-4P
 412284-92-5P 412285-02-0P 412285-03-1P
 412285-05-3P 412285-08-6P 412285-09-7P
 412285-11-1P 412285-12-2P 412285-13-3P
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 412285-17-7P 412285-18-8P 412285-19-9P
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 412288-76-7P 412288-77-8P 412288-78-9P
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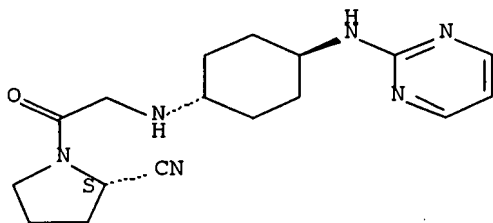
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (S)-N-(N-cyclohexylglycyl)pyrrolidine-2-carbonitriles and (R)-N-(N-cyclohexylglycyl)thiazolidine-2-carbonitriles as dipeptidyl peptidase IV inhibitors for prevention or treatment of diabetes)

RN 412284-89-0 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

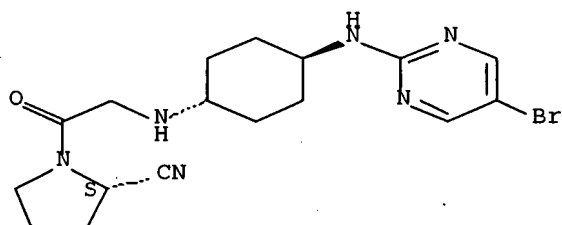


● 2 HCl

RN 412284-90-3 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

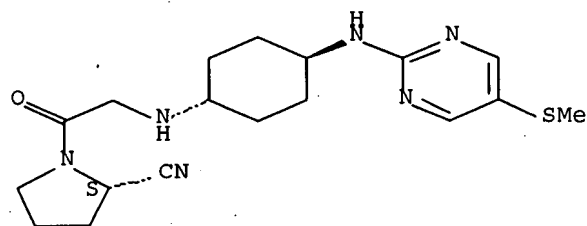


● 2 HCl

RN 412284-91-4 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-(methylthio)-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

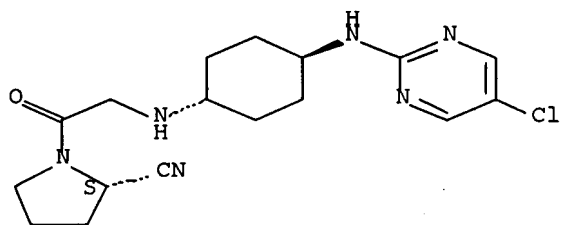


● 2 HCl

RN 412284-92-5 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-chloro-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

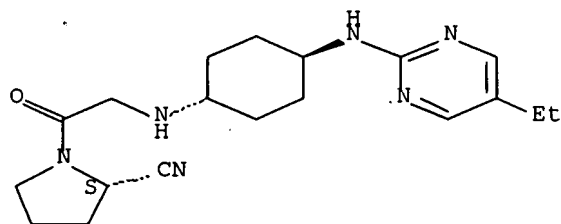


●2 HCl

RN 412285-02-0 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-ethyl-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

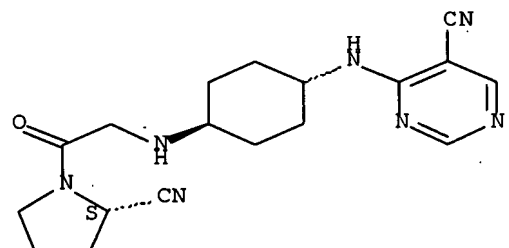


●2 HCl

RN 412285-03-1 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-cyano-4-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

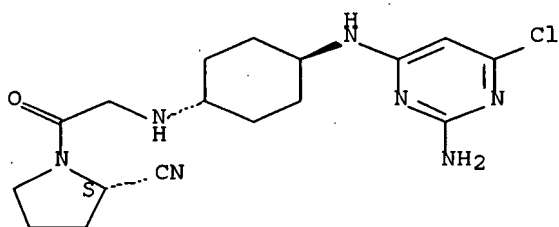


●2 HCl

RN 412285-05-3 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(2-amino-6-chloro-4-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

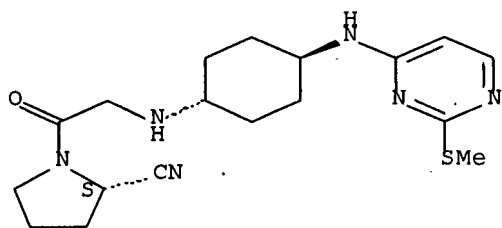


● 2 HCl

RN 412285-08-6 CAPLUS

CN 2-Pyrrolidinecarboxinitrile, 1-[[[trans-4-[[2-(methylthio)-4-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

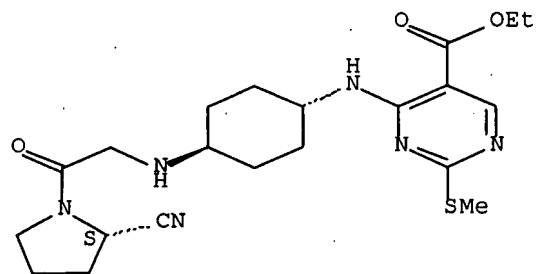


● 2 HCl

RN 412285-09-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(methylthio)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

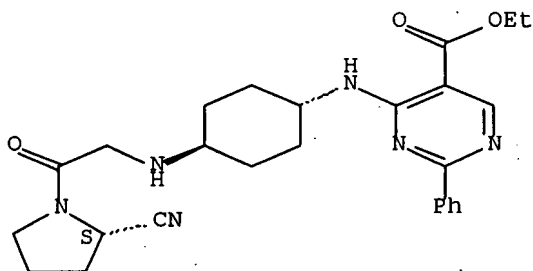


● 2 HCl

RN 412285-11-1 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-phenyl-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

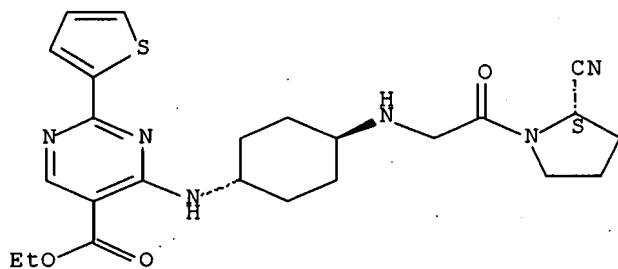


● 2 HCl

RN 412285-12-2 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(2-thienyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

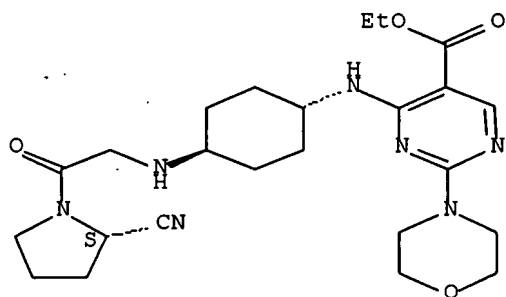


● 2 HCl

RN 412285-13-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(4-morpholinyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

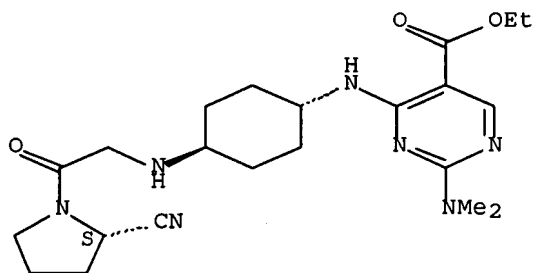


● 2 HCl

RN 412285-14-4 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(dimethylamino)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

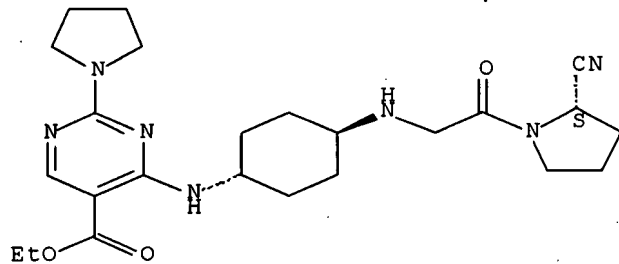


● 2 HCl

RN 412285-15-5 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(1-pyrrolidinyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

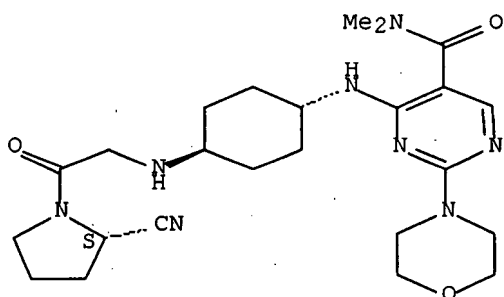


● 2 · HCl

RN 412285-16-6 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-N,N-dimethyl-2-(4-morpholinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

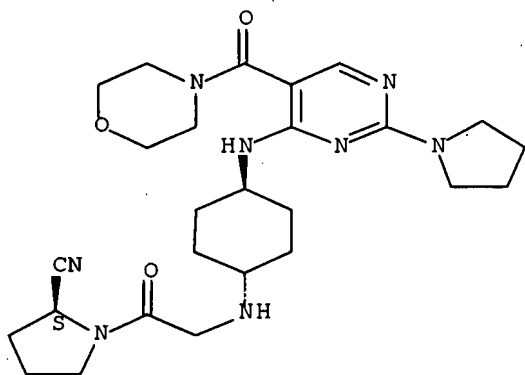


● 2 HCl

RN 412285-17-7 CAPLUS

CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(1-pyrrolidinyl)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

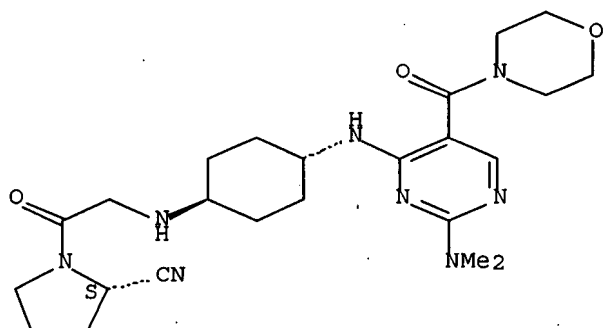


● 2 HCl

RN 412285-18-8 CAPLUS

CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(dimethylamino)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

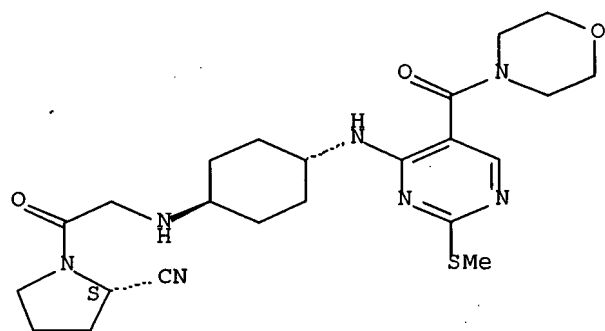


●2 HCl

RN 412285-19-9 CAPLUS

CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(methylthio)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

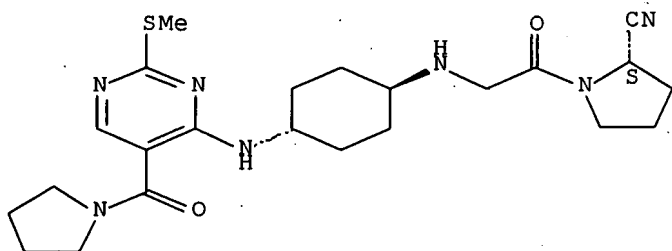


●2 HCl

RN 412285-20-2 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[2-(methylthio)-5-(1-pyrrolidinylcarbonyl)-4-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

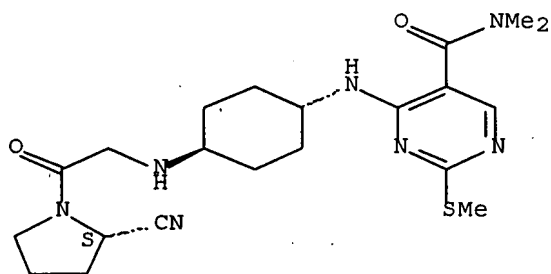


●2 HCl

RN 412285-21-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-N,N-dimethyl-2-(methylthio)-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

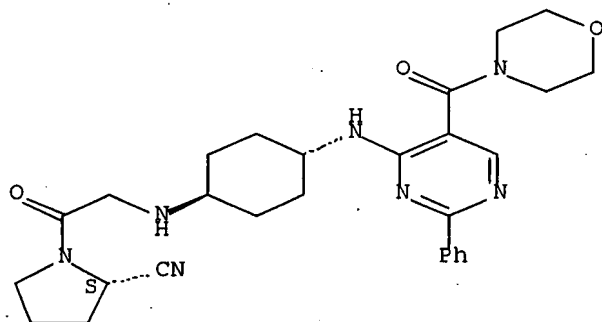


●2 HCl

RN 412285-22-4 CAPLUS

CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-phenyl-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

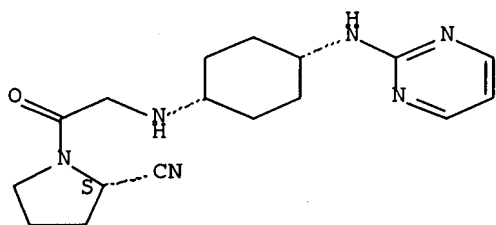


●2 HCl

RN 412285-43-9 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

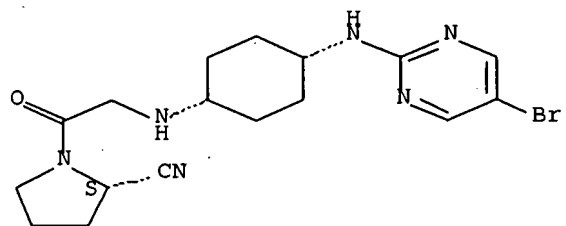


● 2 HCl

RN 412285-44-0 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

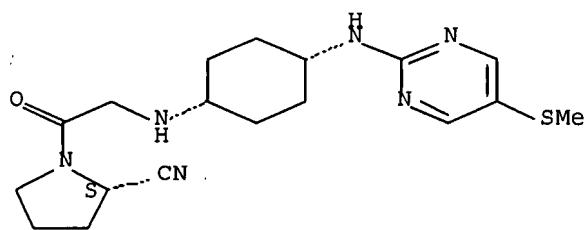


● 2 HCl

RN 412285-45-1 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

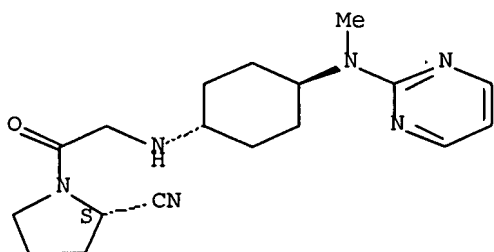


● 2 HCl

RN 412285-64-4 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-(methyl-2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

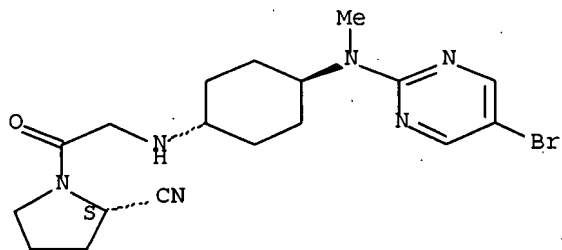


● 2 HCl

RN 412285-65-5 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-bromo-2-pyrimidinyl)methylamino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

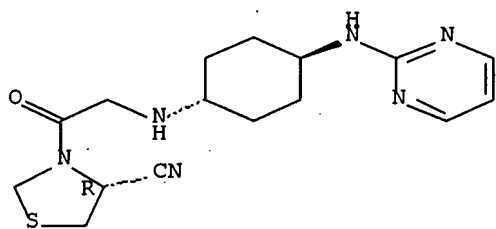


● 2 HCl

RN 412288-75-6 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, monohydrochloride, (4R)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

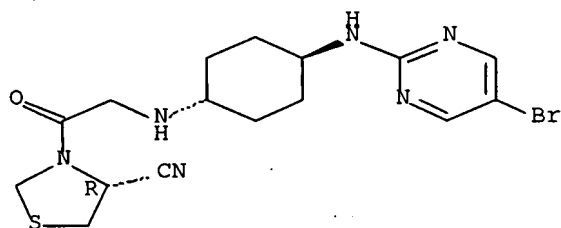


● HCl

RN 412288-76-7 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

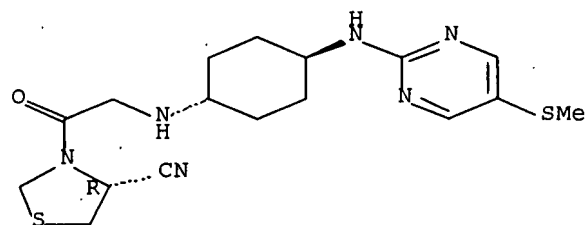


● 2 HCl

RN 412288-77-8 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.



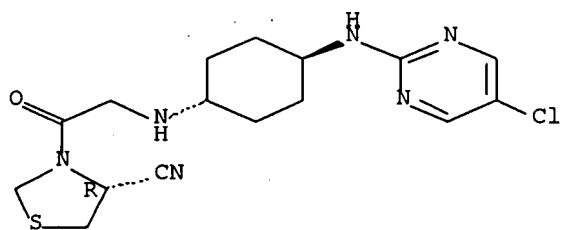
● 2 HCl

RN 412288-78-9 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(5-chloro-2-

pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

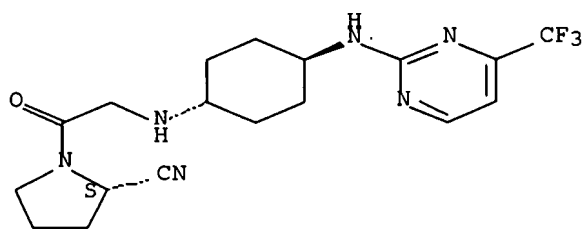


●2 HCl

RN 412915-48-1 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

IT 412294-04-3P

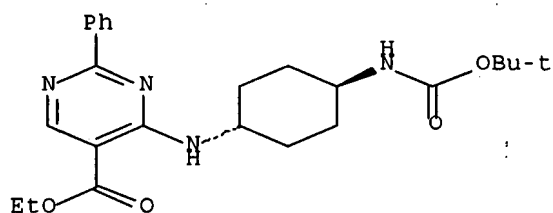
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (S)-N-(N-cyclohexylglycyl)pyrrolidine-2-carbonitriles and (R)-N-(N-cyclohexylglycyl)thiazolidine-2-carbonitriles as dipeptidyl peptidase IV inhibitors for prevention or treatment of diabetes)

RN 412294-04-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[[1,1-dimethylethoxy)carbonyl]amino]cyclohexyl]amino]-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 18 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:293615 CAPLUS Full-text

DOCUMENT NUMBER: 136:325559

TITLE: Preparation of nitrogenous five-membered ring compounds such as (S)-N-[N-cyclohexyl or N-(4-piperidinyl)glycyl]pyrrolidine-2-carbonitrile derivatives as dipeptidyl peptidase IV inhibitors

INVENTOR(S): Yasuda, Kosuke; Morimoto, Hiroshi; Kawanami, Saburo; Hikota, Masataka; Matsumoto, Takeshi; Arakawa, Kenji

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 117 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

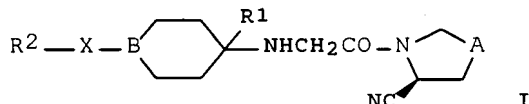
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|------------------|----------------|
| WO 2002030890 | A1 | 20020418 | WO 2001-JP8802 | 20011005 <-- |
| W: AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CO, CR, CU, CZ, DM, DZ, EC, EE, GE, GD, GE, HR, HU, ID, IL, IN, IS, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PH, PL, RO, SG, SI, SK, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2424964 | A1 | 20020418 | CA 2001-2424964 | 20011005 <-- |
| AU 200194196 | A | 20020422 | AU 2001-94196 | 20011005 <-- |
| JP 2002356471 | A | 20021213 | JP 2001-309558 | 20011005 <-- |
| JP 2002356472 | A | 20021213 | JP 2001-309559 | 20011005 <-- |
| EP 1323710 | A1 | 20030702 | EP 2001-974716 | 20011005 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| CN 1468216 | A | 20040114 | CN 2001-816674 | 20011005 <-- |
| NZ 525630 | A | 20041029 | NZ 2001-525630 | 20011005 <-- |
| CN 1891689 | A | 20070110 | CN 2006-10077863 | 20011005 <-- |
| ZA 2003002030 | A | 20030926 | ZA 2003-2030 | 20030313 <-- |
| US 2005054678 | A1 | 20050310 | US 2003-398485 | 20030404 <-- |
| US 7138397 | B2 | 20061121 | | |
| JP 2004035574 | A | 20040205 | JP 2003-368572 | 20031029 <-- |
| AU 2004237882 | A1 | 20050106 | AU 2004-237882 | 20041213 <-- |
| JP 2005200427 | A | 20050728 | JP 2005-105732 | 20050401 <-- |
| AU 2005229666 | A1 | 20051124 | AU 2005-229666 | 20051102 <-- |
| US 2006241146 | A1 | 20061026 | US 2006-452923 | 20060615 <-- |
| PRIORITY APPLN. INFO.: | | | JP 2000-308528 | A 20001006 <-- |

| | |
|----------------|-----------------|
| JP 2000-312562 | A 20001012 <-- |
| JP 2001-99251 | A 20010330 <-- |
| AU 2001-94196 | A3 20011005 <-- |
| CN 2001-816674 | A3 20011005 <-- |
| JP 2001-309558 | A3 20011005 <-- |
| JP 2001-309559 | A3 20011005 <-- |
| WO 2001-JP8802 | W 20011005 <-- |
| US 2003-398485 | A3 20030404 |

OTHER SOURCE(S): MARPAT 136:325559
 ED Entered STN: 19 Apr 2002
 GI



AB Aliphatic nitrogenous five-membered ring compds. of the general formula (I) or pharmacol. acceptable salts thereof [wherein A is CH₂ or S; B is CH or N; R₁ is H, lower alkyl, hydroxy-lower alkyl, lower alkoxy-lower alkyl; X is a single bond, CO, -Alk-CO-, -COCH₂-, -Alk-O-, -O-CH₂-, SO₂, S, CO₂, -CON(R₃)-, -Alk-CON(R₃)-, -CON(R₃)CH₂-, -Alk-CON(R₃)CH₂-, -COCH₂N(R₃)-, -SO₂NR₃-, or NHCH₂; R₃ is H or lower alkyl; Alk is lower alkylene; and R₂ is (1) an optionally substituted mono or bicyclic hydrocarbonyl or heterocyclyl, (2) amino substituted by 1- 2 of optionally substituted lower alkyl, or (3) lower alkyl, carboxy-lower alkyl, lower alkoxy, lower alkenyl, lower alkoxy-lower alkyl, PhO, phenoxy-lower alkyl, or phenyl-lower alkenyl with the proviso that when X is CO, B is N; or when X is a single bond, R₂ is selected from groups listed in (1) and (2)] are prepared These compds. are useful as dipeptidyl peptidase IV inhibitors for the prevention or treatment of diabetes, in particular type II diabetes (no data). Thus, a solution of 100 mg (S)-1-bromoacetyl-2-cyanopyrrolidine and 247 mg 4-amino-1-(2-pyrimidinyl)piperidine in MeOH/MeCN was stirred at room temperature for 15 h to give, after treatment with 2 N HCl/Et₂O, (S)-2-cyano-1-[[[1-(2-pyrimidinyl)piperidin-4-yl]amino]acetyl]pyrrolidine dihydrochloride.

IT 412355-56-7P 412355-59-0P 412355-60-3P
 412355-61-4P 412355-75-0P 412355-76-1P
 412355-77-2P 412355-78-3P

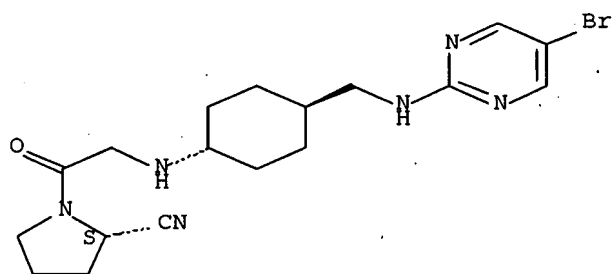
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitrogenous five-membered ring compds. such as (S)-N-glycylpyrrolidinecarbonitrile derivs. as dipeptidyl peptidase IV inhibitors for prevention or treatment of diabetes, in particular type II diabetes)

RN 412355-56-7 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-bromo-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

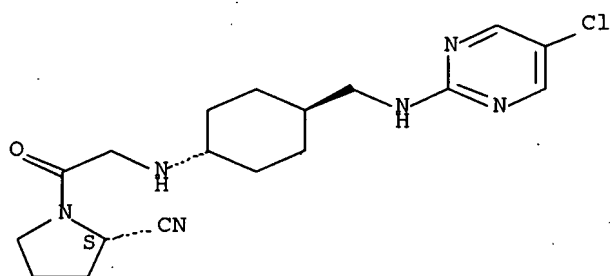


● HCl

RN 412355-59-0 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[[5-chloro-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

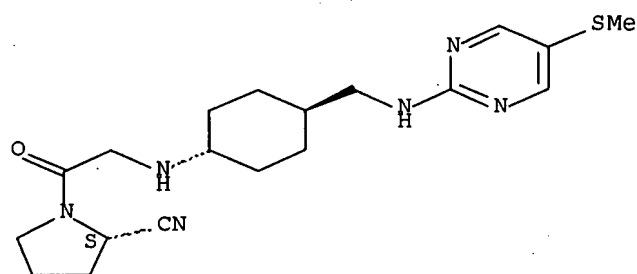


●2 HCl

RN 412355-60-3 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[[5-(methylthio)-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

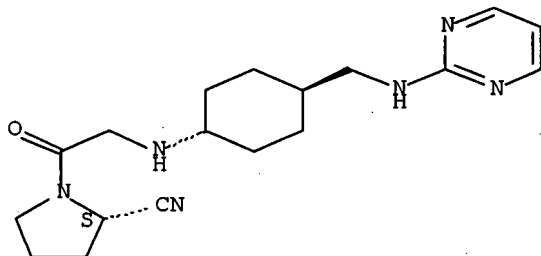


●2 HCl

RN 412355-61-4 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(2-pyrimidinylamino)methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

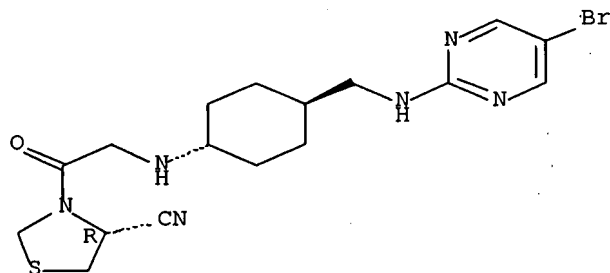


●2 HCl

RN 412355-75-0 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[[5-bromo-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

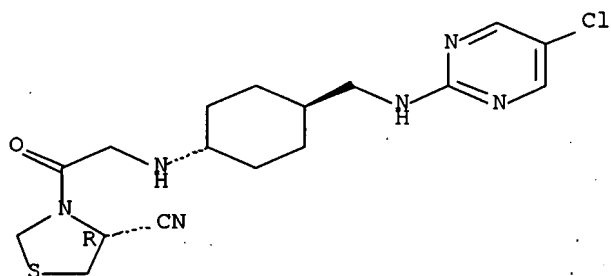


●2 HCl

RN 412355-76-1 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[[5-chloro-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

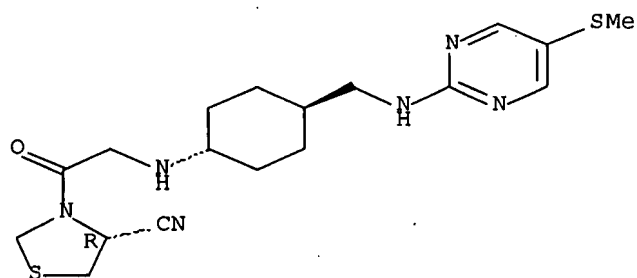


●2 HCl

RN 412355-77-2 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[[5-(methylthio)-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

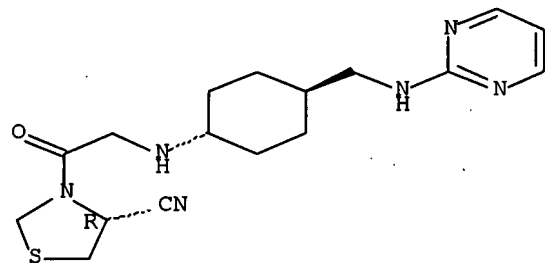


●2 HCl

RN 412355-78-3 CAPLUS

CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(2-pyrimidinylamino)methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)-(9CI) (CA INDEX NAME)

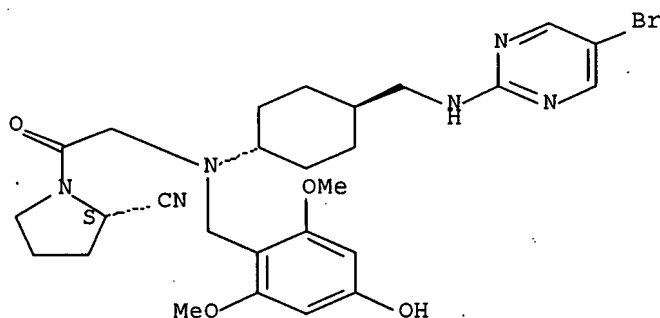
Absolute stereochemistry.



●2 HCl

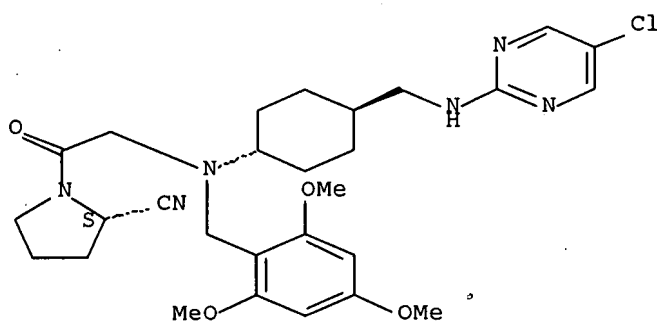
IT 412357-15-4DP, resin-bound 412357-18-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of nitrogenous five-membered ring compds. such as
 (S)-N-glycylpyrrolidinecarbonitrile derivs. as dipeptidyl peptidase IV
 inhibitors for prevention or treatment of diabetes, in particular type
 II diabetes)
 RN 412357-15-4 CAPLUS
 CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[5-bromo-2-
 pyrimidinyl)amino]methyl]cyclohexyl][(4-hydroxy-2,6-
 dimethoxyphenyl)methyl]amino]acetyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 412357-18-7 CAPLUS
 CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[5-chloro-2-
 pyrimidinyl)amino]methyl]cyclohexyl][(2,4,6-trimethoxyphenyl)methyl]amino]
 acetyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 19 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:923757 CAPLUS Full-text

DOCUMENT NUMBER: 136:37503

TITLE: Preparation of N-glycyl-2-cyanopyrrolidines as DPP IV
 inhibitors

INVENTOR(S): Villhauer, Edwin Bernard

PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis-Erfindungen
 Verwaltungsgesellschaft m.b.H.

SOURCE: PCT Int. Appl., 50 pp.

CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|------------------|-----------------|
| WO 2001096295 | A2 | 20011220 | WO 2001-EP6595 | 20010611 <-- |
| WO 2001096295 | A3 | 20020516 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| TW 583185 | B | 20040411 | TW 2001-90113972 | 20010608 <-- |
| CA 2411778 | A1 | 20011220 | CA 2001-2411778 | 20010611 <-- |
| EP 1296974 | A2 | 20030402 | EP 2001-984014 | 20010611 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| JP 2004503531 | T | 20040205 | JP 2002-510439 | 20010611 <-- |
| US 6432969 | B1 | 20020813 | US 2001-879654 | 20010612 <-- |
| US 2002193390 | A1 | 20021219 | US 2002-176440 | 20020620 <-- |
| PRIORITY APPLN. INFO.: | | | US 2000-325743P | P 20000613 <-- |
| | | | US 2000-592336 | A 20000613 <-- |
| | | | WO 2001-EP6595 | W 20010611 <-- |
| | | | US 2001-879654 | A3 20010612 <-- |

OTHER SOURCE(S): MARPAT 136:37503

ED Entered.STN: 21 Dec 2001

AB The present invention relates to the preparation of N-(substituted glycy)-2-cyanopyrrolidines. Thus, 1-chloroacetyl-2-(S)-cyanopyrrolidine (synthetic preparation given) is reacted with 2-[(5-chloro-2-pyridinyl)amino]-1,1-dimethylethylamine in the presence of K₂CO₃ to give 1-[[[2-[(5-chloro-2-pyridinyl)amino]-1,1-dimethylethyl]amino]acetyl]-2-cyano-(S)-pyrrolidine. The prepared compds. inhibit DPP-IV (dipeptidyl-peptidase-IV) activity. They are therefore indicated for use as pharmaceuticals in inhibiting DPP-IV and in the treatment of conditions mediated by DPP-IV, such as non-insulin-dependent diabetes mellitus, arthritis, obesity, osteoporosis and further conditions of impaired glucose tolerance. Data for biol. activity of some of the prepared compds. were given.

IT 380831-65-2P 380831-69-6P

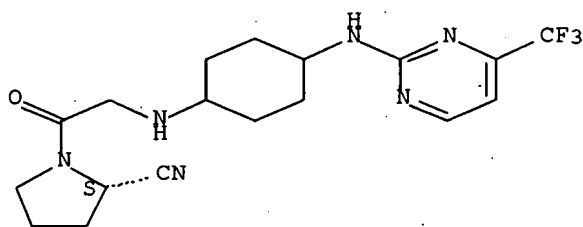
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-glycyl-2-cyanopyrrolidines as DPP IV inhibitors)

RN 380831-65-2 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[4-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI)
 (CA INDEX NAME)

Absolute stereochemistry.

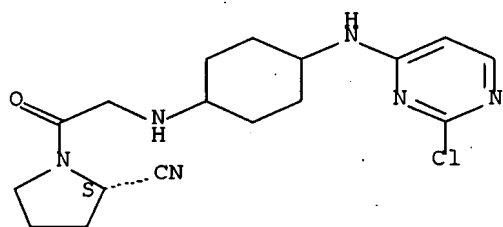


● 2 HCl

RN 380831-69-6 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[4-[(2-chloro-4-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.



● 2 HCl

L23 ANSWER 20 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:900621 CAPLUS Full-text

DOCUMENT NUMBER: 134:56683

TITLE: Preparation of nitrogen-containing heterocyclic derivatives as remedies for complications of diabetes based on protein kinase C inhibition

INVENTOR(S): Suzuki, Takayuki; Onda, Kenichi; Murakami, Takeshi; Negoro, Kenji; Yahiro, Kiyoshi; Maruyama, Tatsuya; Shimaya, Akiyoshi; Ohta, Mitsuaki

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 62 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| WO 2000076980 | A1 | 20001221 | WO 2000-JP3768 | 20000609 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, | | | | |

ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
 CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

JP 1999-163344

A 19990610 <--

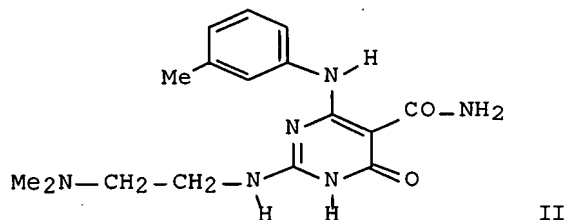
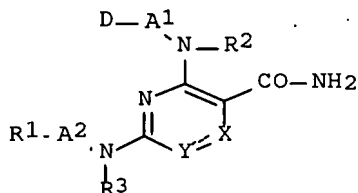
JP 1999-165217

A 19990611 <--

OTHER SOURCE(S): MARPAT 134:56683

ED Entered STN: 22 Dec 2000.

GI



AB The title compds. I [Y and X together are N:N, C(R4):N, etc.; D = (un)substituted aryl, etc.; R1 = (un)substituted heteroaryl, etc.; A1, A2 = (un)substituted alkylene, etc.; R2, R3, R4 = H, OH, etc.; or R1A2NR3 = (un)substituted heteroaryl] are prepared. The title compound II in vitro showed IC50 of 0.0049 μ mol against protein kinase C.

IT 313337-98-3P 313337-99-4P 313338-14-6P
 313338-15-7P 313338-42-0P 313338-55-5P
 313338-56-6P

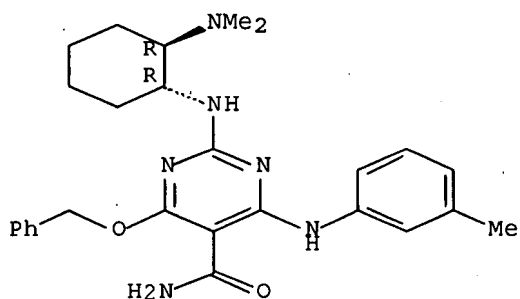
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitrogen-containing heterocyclic derivs. as remedies for complications of diabetes)

RN 313337-98-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[[(1R,2R)-2-(dimethylamino)cyclohexyl]amino]-4-[(3-methylphenyl)amino]-6-(phenylmethoxy)]- (9CI) (CA INDEX NAME)

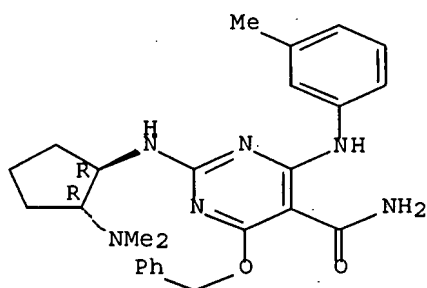
Absolute stereochemistry.



RN 313337-99-4 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[[(1R,2R)-2-(dimethylamino)cyclopentyl]amino]-4-[(3-methylphenyl)amino]-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)

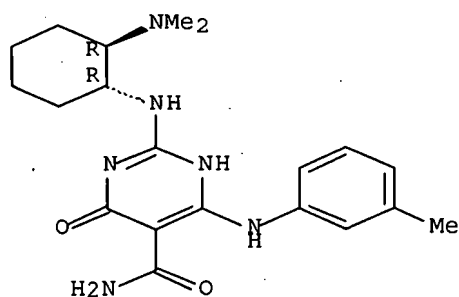
Absolute stereochemistry.



RN 313338-14-6 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[[(1R,2R)-2-(dimethylamino)cyclohexyl]amino]-1,4-dihydro-6-[(3-methylphenyl)amino]-4-oxo- (9CI) (CA INDEX NAME)

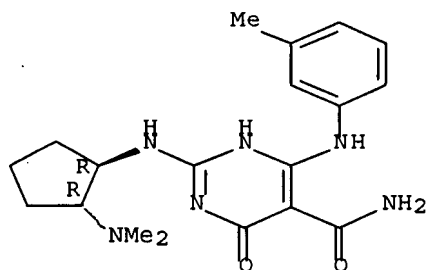
Absolute stereochemistry.



RN 313338-15-7 CAPLUS

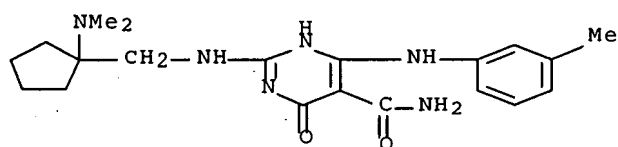
CN 5-Pyrimidinecarboxamide, 2-[[[(1R,2R)-2-(dimethylamino)cyclopentyl]amino]-1,4-dihydro-6-[(3-methylphenyl)amino]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 313338-42-0 CAPLUS

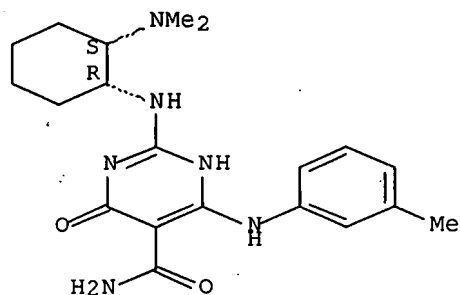
CN 5-Pyrimidinecarboxamide, 2-[[[1-(dimethylamino)cyclopentyl]methyl]amino]-1,4-dihydro-6-[(3-methylphenyl)amino]-4-oxo- (9CI) (CA INDEX NAME)



RN 313338-55-5 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[[(1R,2S)-2-(dimethylamino)cyclohexyl]amino]-1,4-dihydro-6-[(3-methylphenyl)amino]-4-oxo- (9CI) (CA INDEX NAME)

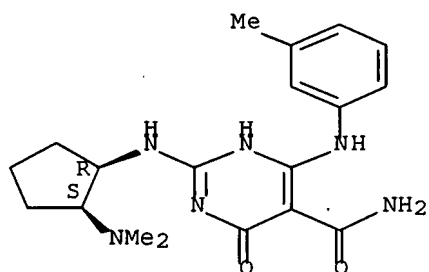
Absolute stereochemistry:



RN 313338-56-6 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[[(1R,2S)-2-(dimethylamino)cyclopentyl]amino]-1,4-dihydro-6-[(3-methylphenyl)amino]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



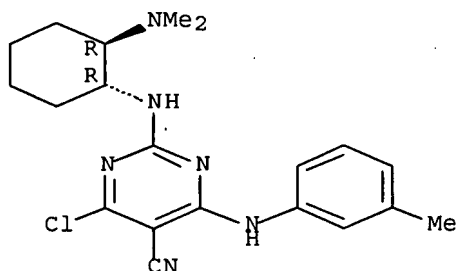
IT 313339-17-2P 313339-18-3P 313339-27-4P
313339-28-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of nitrogen-containing heterocyclic derivs. as remedies for
complications of diabetes)

RN 313339-17-2 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-chloro-2-[[[(1R,2R)-2-(
(dimethylamino)cyclohexyl]amino]-6-[(3-methylphenyl)amino]- (9CI) (CA
INDEX NAME)

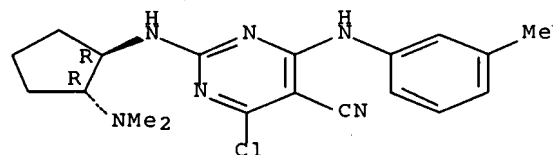
Absolute stereochemistry.



RN 313339-18-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-chloro-2-[[[(1R,2R)-2-(
(dimethylamino)cyclopentyl]amino]-6-[(3-methylphenyl)amino]- (9CI) (CA
INDEX NAME)

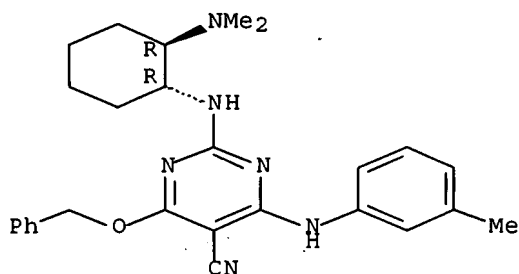
Absolute stereochemistry.



RN 313339-27-4 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-[[[(1R,2R)-2-(dimethylamino)cyclohexyl]amino]-4-
[(3-methylphenyl)amino]-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)

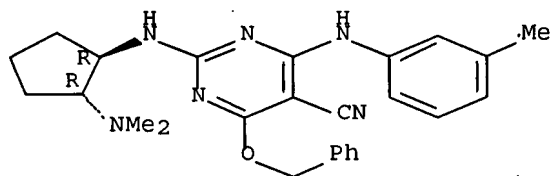
Absolute stereochemistry.



RN 313339-28-5 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-[[[(1R,2R)-2-(dimethylamino)cyclopentyl]amino]-4-[(3-methylphenyl)amino]-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 21 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:881124 CAPLUS Full-text

DOCUMENT NUMBER: 134:42141

TITLE: Preparation of novel heterocyclic carboxamide derivatives as spleen tyrosine kinase inhibitors
INVENTOR(S): Hisamichi, Hiroyuki; Kawazoe, Souichirou; Tanabe, Kazuhito; Ichikawa, Atsushi; Orita, Akiko; Suzuki, Takayuki; Onda, Kenichi; Takeuchi, Makoto

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 36 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| WO 2000075113 | A1 | 20001214 | WO 2000-JP3767 | 20000609 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| JP 2001055378 | A | 20010227 | JP 2000-171185 | 20000607 <-- |

| | | | | |
|---|----|----------|----------------|--------------|
| EP 1184376 | A1 | 20020306 | EP 2000-935619 | 20000609 <-- |
| EP 1184376 | B1 | 20050202 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| AT 288420 | T | 20050215 | AT 2000-935619 | 20000609 <-- |
| PT 1184376 | T | 20050429 | PT 2000-935619 | 20000609 <-- |
| ES 2237430 | T3 | 20050801 | ES 2000-935619 | 20000609 <-- |
| US 6797706 | B1 | 20040928 | US 2001-9276 | 20011210 <-- |

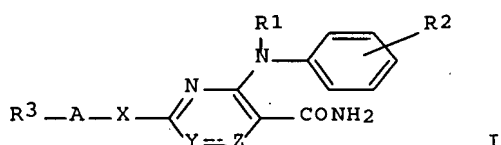
PRIORITY APPLN. INFO.:

| | | |
|----------------|---|--------------|
| JP 1999-162692 | A | 19990609 <-- |
| WO 2000-JP3767 | W | 20000609 <-- |

OTHER SOURCE(S): MARPAT 134:42141

ED Entered STN: 15 Dec 2000

GI



AB Nitrogenous six-membered heterocycle compds. bearing as the substituents -X-A-R₃, -N-(R₁)-(R₂-substituted Ph) and -CONH₂ [I; wherein A = (substituted) lower alkylene, (substituted) (hetero)arylene, cycloalkylene; X = NR₄, CONR₄, NR₄CO, O, S; the dotted line between Y and Z represents the presence of a bond (Y:Z) or the absence of a bond (Y-Z); Y-Z = NR₅-CO, CO-NR₅, NR₅-NR₅, CO-CO; Y:Z = N:CR₁, CR₇:N, N:N, CR₇:CR₇; R₄ = each H, lower alkyl, -CO-lower alkyl, or -SO₂-lower alkyl; R₂ = H, (halo-substituted) lower alkyl, -O-lower alkyl, -S-lower alkyl, -O-aryl, nitro, cyano, or the like; R₃ = -CO₂H, -CO₂-lower alkyl, -lower alkylene-CO₂H, -NH₂, -alkylene-NH₂, or the like; R₅ = H, lower alkyl; R₆ = lower alkyl, OH, -O-lower alkyl, -O-(substituted) aryl, -O-lower alkylene-(substituted) aryl, -NR₁-(substituted) aryl, -CO-lower alkyl-(substituted) aryl; R₇ = H, R₆] salts or prodrugs thereof are prepared Also claimed are spleen tyrosine kinase (Syk) inhibitors containing the compds. I or the salts or the prodrugs thereof as the active ingredient. The compds. I are useful for the prevention or treatment of allergies, inflammations, autoimmune diseases, cancers, transplant rejection, graft-vs.-host diseases, and thrombosis. Thus, 2.76 mL cis-1,2-cyclohexanediamine was added to a mixture of 605 mg 6-chloro-2-(3-methylanilino)pyridine-3-carboxamide and 10 mL MeCN and refluxed for 5 days to give 230 mg 6-(cis-2-aminohexylamino)-2-(3-methylanilino)pyrazine-3-carboxamide (II). II showed IC₅₀ of ≤0.05 μM against Syk, good inhibition against passive cutaneous anaphylaxis (PCA) in mice sensitized by anti-dinitrophenyl-IgE (DNP-IgE), and IC₅₀ of ≤0.1 μM against serotonin release according to the assay described by Collado-Escobar (J. Immunol. 144, 1990).

IT 312736-54-2 312736-56-4

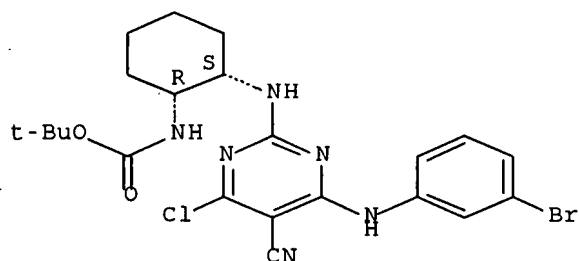
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of novel heterocyclic carboxamide derivs. as spleen tyrosine kinase inhibitors as preventives or remedies for diseases)

RN 312736-54-2 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-[(3-bromophenyl)amino]-6-chloro-5-cyano-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

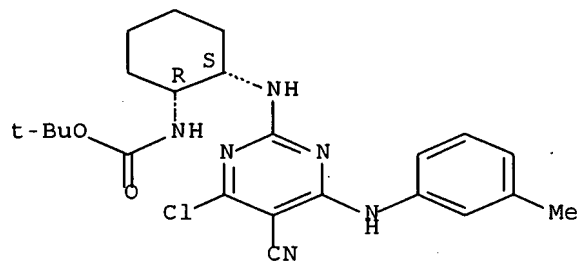
Relative stereochemistry.



RN 312736-56-4 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-chloro-5-cyano-6-[(3-methylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 312736-55-3P 312736-63-3P 312736-78-0P

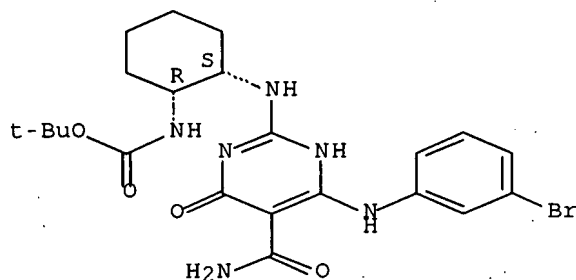
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of novel heterocyclic carboxamide derivs. as spleen tyrosine kinase inhibitors as preventives or remedies for diseases)

RN 312736-55-3 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[5-(aminocarbonyl)-6-[(3-bromophenyl)amino]-1,4-dihydro-4-oxo-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

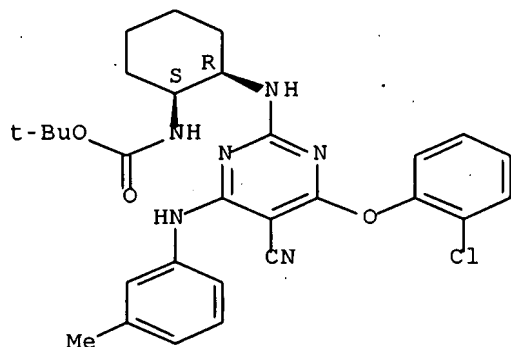
Relative stereochemistry.



RN 312736-63-3 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[4-(2-chlorophenoxy)-5-cyano-6-[(3-methylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

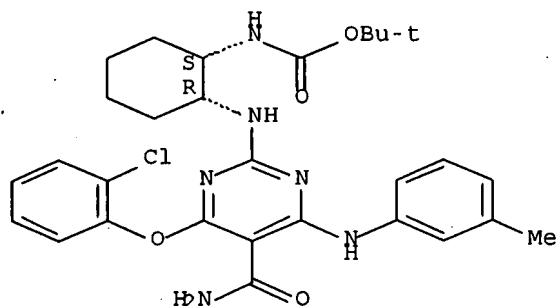
Relative stereochemistry.



RN 312736-78-0 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[5-(aminocarbonyl)-4-(2-chlorophenoxy)-6-[(3-methylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 22 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:241135 CAPLUS Full-text

DOCUMENT NUMBER: 132:279106

TITLE: Non-peptide GnRH agents, methods and intermediates for their preparation

INVENTOR(S): Anderson, Mark Brian; Vazir, Haresh N.; Luthin, David Robert; Paderes, Genevieve Deguzman; Pathak, Ved P.; Christie, Lance Christopher; Hong, Yufeng; Tompkins, Eileen Valenzuela; Li, Haitao; Faust, James

PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA; et al.

SOURCE: PCT Int. Appl., 444 pp.

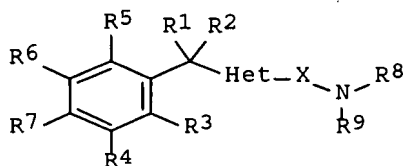
CODEN: PIXXD2

DOCUMENT TYPE: Patent

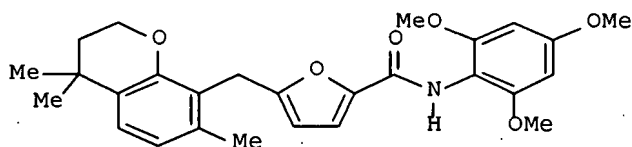
LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-------------------|-----------------|
| WO 2000020358 | A2 | 20000413 | WO 1999-US18790 | 19990820 <-- |
| WO 2000020358 | A3 | 20001116 | | |
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| RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2341346 | A1 | 20000413 | CA 1999-2341346 | 19990820 <-- |
| BR 9913374 | A | 20010515 | BR 1999-13374 | 19990820 <-- |
| EP 1105120 | A2 | 20010613 | EP 1999-968010 | 19990820 <-- |
| EP 1105120 | B1 | 20050323 | | |
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| HU 200103622 | A2 | 20020429 | HU 2001-3622 | 19990820 <-- |
| EE 200100102 | A | 20020617 | EE 2001-102 | 19990820 <-- |
| SI 20746 | A | 20020630 | SI 1999-20076 | 19990820 <-- |
| TR 200100631 | T2 | 20020821 | TR 2001-200100631 | 19990820 <-- |
| JP 2002535244 | T | 20021022 | JP 2000-574479 | 19990820 <-- |
| AU 759310 | B2 | 20030410 | AU 2000-24709 | 19990820 <-- |
| NZ 509252 | A | 20040528 | NZ 1999-509252 | 19990820 <-- |
| AT 291423 | T | 20050415 | AT 1999-968010 | 19990820 <-- |
| ES 2237966 | T3 | 20050801 | ES 1999-968010 | 19990820 <-- |
| NO 2001000309 | A | 20010411 | NO 2001-309 | 20010119 <-- |
| IN 2001DN00066 | A | 20070112 | IN 2001-DN66 | 20010124 <-- |
| ZA 2001000831 | A | 20020822 | ZA 2001-831 | 20010130 <-- |
| MX 2001PA01834 | A | 20000821 | MX 2001-PA1834 | 20010219 <-- |
| US 7101878 | B1 | 20060905 | US 2001-763216 | 20010220 <-- |
| LV 12732 | B | 20020320 | LV 2001-45 | 20010316 <-- |
| BG 105362 | A | 20011231 | BG 2001-105362 | 20010319 <-- |
| LT 4904 | B | 20020425 | LT 2001-24 | 20010319 <-- |
| US 2004010033 | A1 | 20040115 | US 2003-353160 | 20030708 <-- |
| PRIORITY APPLN. INFO.: | | | US 1998-97520P | P 19980820 <-- |
| | | | WO 1999-US18790 | W 19990820 <-- |
| | | | US 2001-763216 | B3 20010220 <-- |

OTHER SOURCE(S): MARPAT 132:279106
 ED Entered STN: 14 Apr 2000
 GI



I



II

AB Non-peptide GnRH agents capable of inhibiting the effect of gonadotropin-releasing hormone are described. The compds. and their pharmaceutically acceptable salts, multimers, prodrugs, and active metabolites are suitable for treating mammalian reproductive disorders and steroid hormone-dependent tumors as well as for regulating fertility, where suppression of gonadotropin release is indicated. The compds. include those of formula I [X = C:O, C:S, S:O, or SO₂; Het = 5-membered NOS-heterocycle; R₁, R₂ = H, alkyl; R₃-R₇ = H, halo, (un)substituted alkyl, aryl, heteroaryl, CH₂OR, OR, CO₂R; R = alkyl, aryl, etc.; adjacent rings positions such as R₆R₇ may form (un)substituted 5- or 6-membered ring with up to 4 heteroatoms; R₈ = lipophilic moiety such as alkyl, aryl, CH₂OR, OR, etc.; R₉ = H, (un)substituted alkyl]. Methods and intermediates for synthesizing the compds. are also described. For instance, 4,4,7-trimethylchroman (preparation given) was alkylated in the 6- and 8-positions using Et 5-(chloromethyl)-2-furoate (46% total yield), and the resulting esters were hydrolyzed to a mixture of acids. This unsepd. mixture was treated with SOCl₂ and amidated with 2,4,6-trimethoxyphenylamine-HCl to give the invention compound II and its chroman-6-position isomer, which were separated by HPLC. Several compds. exhibited high affinity (<100 nM) at human GnRH receptors. The compds. antagonized GnRH-stimulated inositol phosphate accumulation in cells with recombinant human GnRH receptors, and an example compound reduced plasma LH levels in castrated male rats. Various biol. data for several hundred compds. are given.

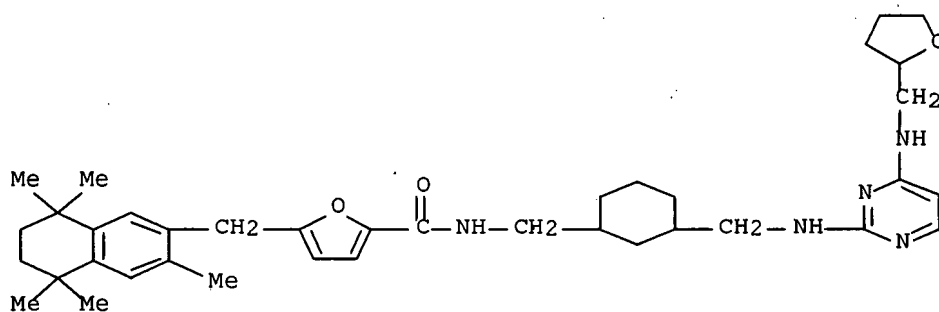
IT 263847-63-8P 263848-23-3P 263848-26-6P
263848-44-8P 263848-45-9P 263848-46-0P
263848-62-0P 263848-88-0P 263849-03-2P
263849-24-7P 263849-27-0P 263851-05-4P
263854-72-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of non-peptide GnRH agents for regulating gonadotropin secretion)

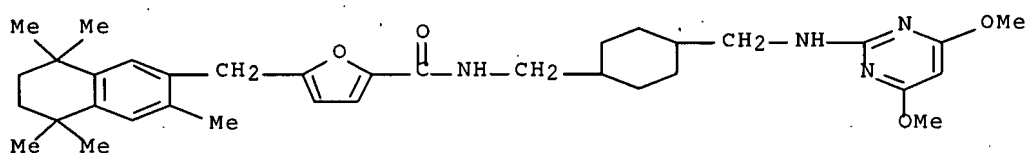
RN 263847-63-8 CAPLUS

CN 2-Furancarboxamide, N-[[3-[[[4-[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



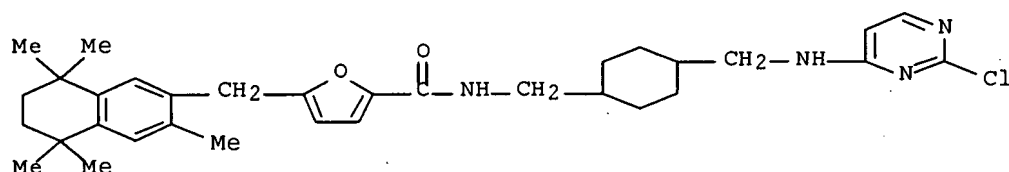
RN 263848-23-3 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[(4,6-dimethoxy-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]]- (9CI) (CA INDEX NAME)



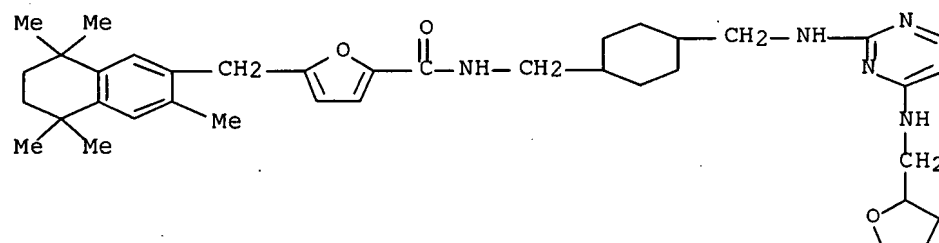
RN 263848-26-6 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[(2-chloro-4-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]]- (9CI) (CA INDEX NAME)



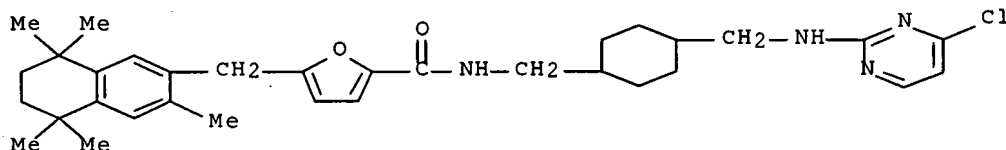
RN 263848-44-8 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[(4-[[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]]- (9CI) (CA INDEX NAME)



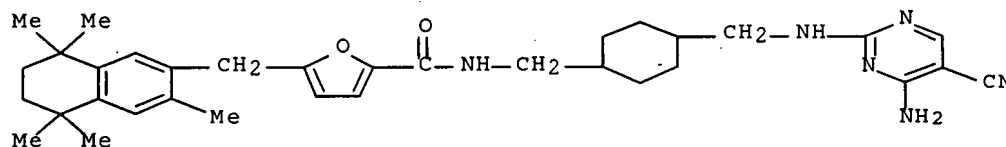
RN 263848-45-9 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[(4-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



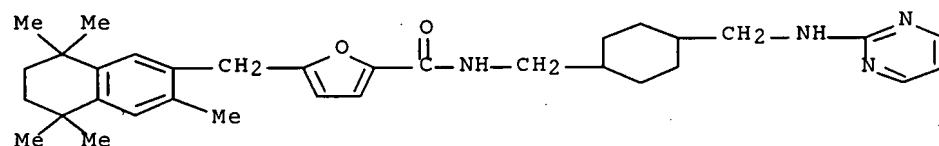
RN 263848-46-0 CAPLUS

CN 2-Furancarboxamide, N-[[4-[[[(4-amino-5-cyano-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



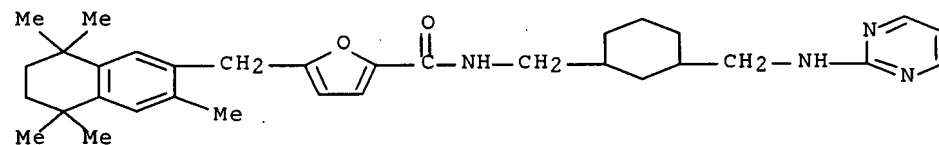
RN 263848-62-0 CAPLUS

CN 2-Furancarboxamide, N-[[4-[(2-pyrimidinylamino)methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



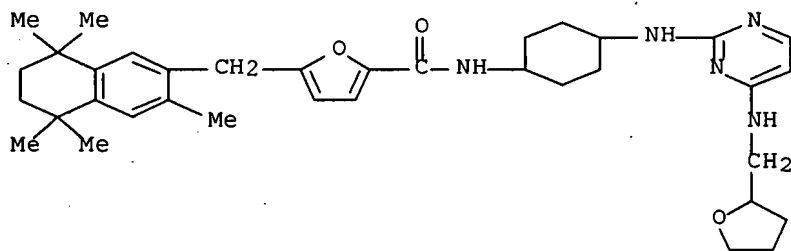
RN 263848-88-0 CAPLUS

CN 2-Furancarboxamide, N-[[3-[(2-pyrimidinylamino)methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



RN 263849-03-2 CAPLUS

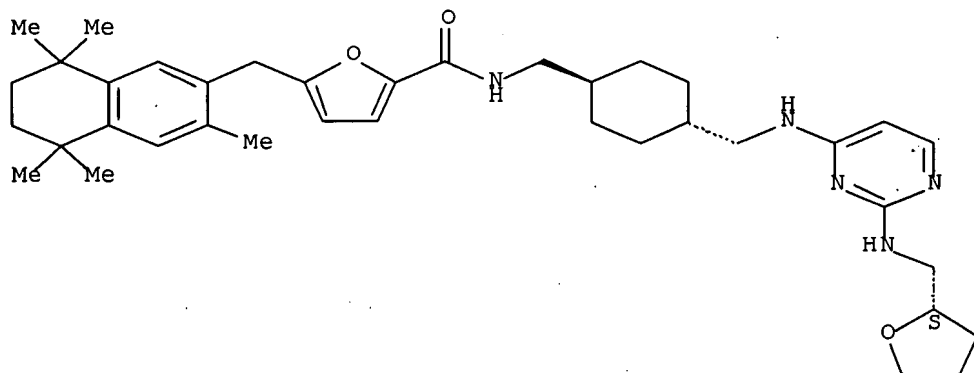
CN 2-Furancarboxamide, N-[4-[[4-[[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]cyclohexyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



RN 263849-24-7 CAPLUS

CN 2-Furancarboxamide, N-[[trans-4-[[[2-[[[(2S)-tetrahydro-2-furanyl)methyl]amino]-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

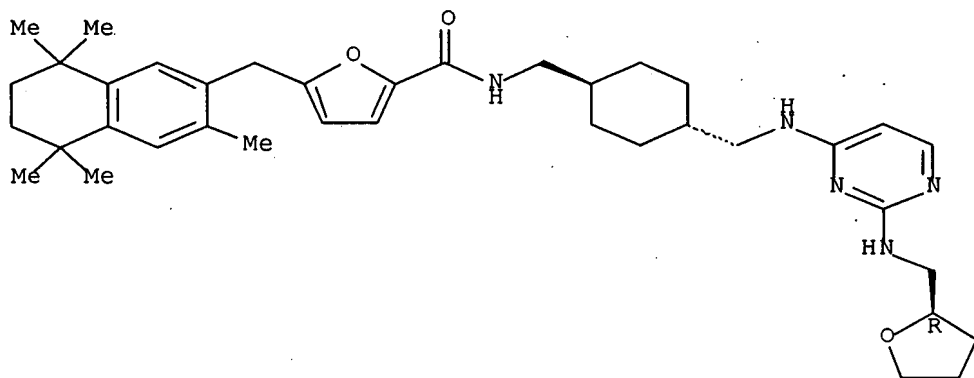
Absolute stereochemistry.



RN 263849-27-0 CAPLUS

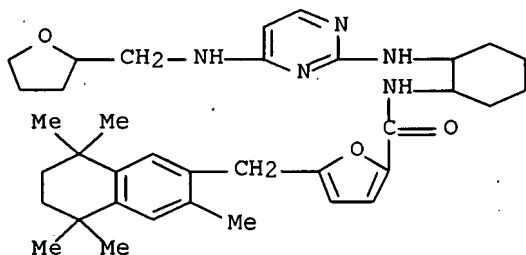
CN 2-Furancarboxamide, N-[[trans-4-[[[2-[[[(2R)-tetrahydro-2-furanyl)methyl]amino]-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



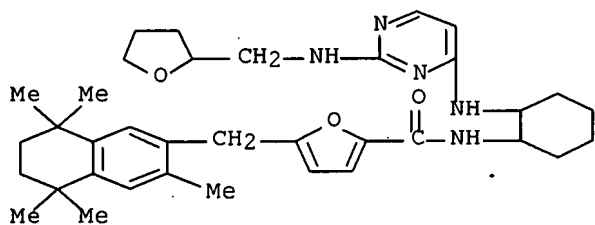
RN 263851-05-4 CAPLUS

CN 2-Furancarboxamide, N-[2-[[4-[[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]cyclohexyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



RN 263854-72-4 CAPLUS

CN 2-Furancarboxamide, N-[2-[[2-[[[(tetrahydro-2-furanyl)methyl]amino]-4-pyrimidinyl]amino]cyclohexyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



L23 ANSWER 23 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:33829 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 132:193982

TITLE: Self-assembly of helical supramolecular channels from chiral aminopyrimidine hydrogen bonding motifs in the solid state

AUTHOR(S): Krische, Michael J.; Lehn, Jean-Marie; Cheung, Eugene;

Vaughn, Gavin; Krische, Amy L.
 CORPORATE SOURCE: Laboratoire de chimie supramoléculaire, CNRS ESA 7006, ISIS, CNRS ESA 7006, ISIS, universite Louis-Pasteur, Strasbourg, 67000, Fr.
 SOURCE: Comptes Rendus de l'Academie des Sciences, Serie IIc: Chimie (1999), 2(11-13), 549-556
 CODEN: CASCEN; ISSN: 1387-1609
 PUBLISHER: Editions Scientifiques et Medicales Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 14 Jan 2000
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

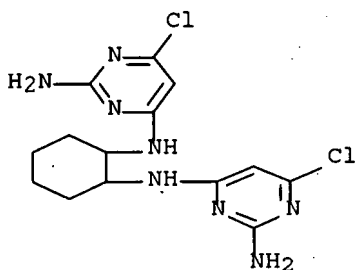
AB The H-bond mediated self-assembly of the chiral C2-sym. bis-(2-amino-4-chloro-pyrimidines) I and II allows for the mol. recognition directed generation of helical superstructures. In the former case, unoccupied channel structures defined by the cylindrical interior of the derived supramol. helix result, as revealed by X-ray crystallog. anal. using a synchrotron source. Upon crystallization, racemic I spontaneously resolves to form homochiral crystals exhibiting a helical packing motif identical to that determined for optically pure I. The data provide insight into the interplay of the different structural and interactional features of the mol. components to the generation of the channel structure and suggest design strategies toward porous organic mol. solids of variable size.

IT 259675-38-2P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
 (racemate; self-assembly of helical supramol. channels from chiral aminopyrimidine hydrogen bonding motifs in the solid state)

RN 259675-38-2 CAPLUS

CN 2,4-Pyrimidinediamine, N4,N4'-1,2-cyclohexanediylbis[6-chloro- (9CI) (CA INDEX NAME)



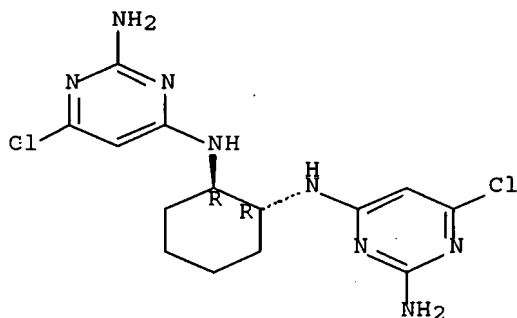
IT 259675-37-1P

RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
 (self-assembly of helical supramol. channels from chiral aminopyrimidine hydrogen bonding motifs in the solid state)

RN 259675-37-1 CAPLUS

CN 2,4-Pyrimidinediamine, N4,N4'-(1R,2R)-1,2-cyclohexanediylbis[6-chloro- (9CI) (CA INDEX NAME)

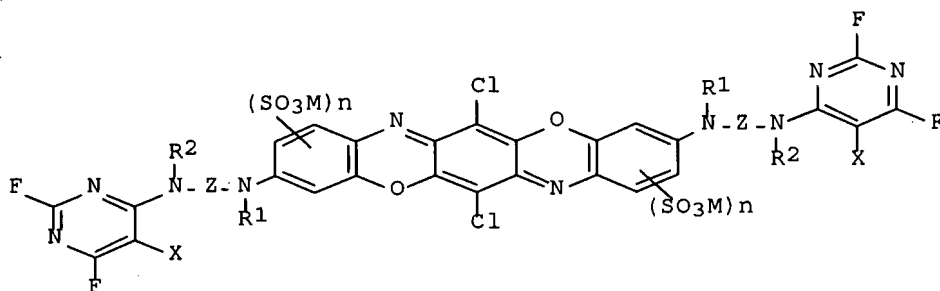
Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 24 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1999:791797 CAPLUS Full-text
 DOCUMENT NUMBER: 132:23860
 TITLE: Water-soluble triphenyldioxazine reactive dyes, their production and their use
 INVENTOR(S): Reiher, Uwe; Brandl, Matthias
 PATENT ASSIGNEE(S): DyStar Textilfarben G.m.b.H. und Co. Deutschland
 K.-G., Germany
 SOURCE: Ger. Offen., 10 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------------------|------|----------|------------------|--------------|
| DE 19824663 | A1 | 19991209 | DE 1998-19824663 | 19980603 <-- |
| PRIORITY APPLN. INFO.: | | | DE 1998-19824663 | 19980603 <-- |
| OTHER SOURCE(S): MARPAT 132:23860 | | | | |
| ED Entered STN: 16 Dec 1999 | | | | |
| GI | | | | |



I

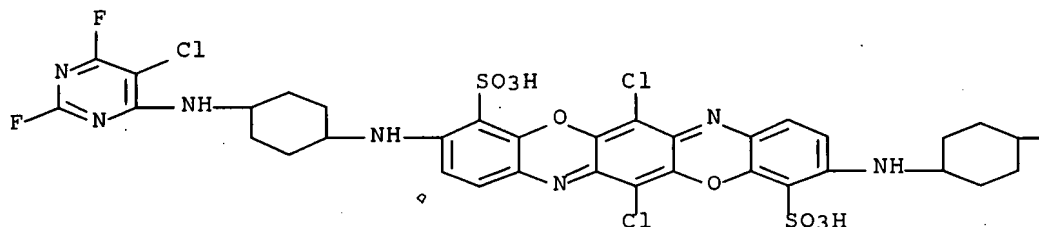
AB The fluoropyrimidine reactive dyes (I; R1, R2 = H, optionally substituted C1-4-alkyl; X = Cl, H; Z = organic connecting group; n = 1, 2) are obtained from triphenodioxazine diamine derivs. and fluoropyrimidines and provide fast blue dyeings on textiles, especially cotton. In an example, I (R1 = R2 = X = H; Z = CH2CH2; n = 1) (λ_{\max} 620) is obtained from 2,4,6-trifluoropyrimidine and the appropriate diamine.

IT 252014-68-9P
 RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
 (blue dye; production of water-soluble triphenodioxazine reactive dyes for cotton)

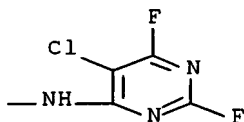
RN 252014-68-9 CAPLUS

CN 4,11-Triphenodioxazinedisulfonic acid, 6,13-dichloro-3,10-bis[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]cyclohexyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L23 ANSWER 25 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:404941 CAPLUS Full-text

DOCUMENT NUMBER: 131:44844

TITLE: preparation of novel pyrimidine-5-carboxamide derivatives as tyrosinase inhibitors

INVENTOR(S): Hisamichi, Hiroyuki; Naito, Ryo; Kawazoe, Souichirou; Toyoshima, Akira; Tanabe, Kazuhito; Nakai, Eiichi; Ichikawa, Atsushi; Orita, Akiko; Takeuchi, Makoto

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 43 pp.
 CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

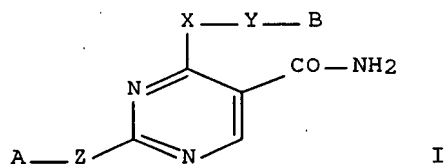
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|-------|-------|-----------------|-------|
| ----- | ----- | ----- | ----- | ----- |

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WO 9931073          A1      19990624      WO 1998-JP5643          19981214 <--
W:  AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH,
    GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
    LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI,
    SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY,
    KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
    FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
    CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
AU 9915071          A      19990705      AU 1999-15071          19981214 <--
EP 1054004          A1      20001122      EP 1998-959197          19981214 <--
R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI
US 6432963          B1      20020813      US 2000-581595          20000615 <--
PRIORITY APPLN. INFO.:          JP 1997-344588          A 19971215 <--
                                WO 1998-JP5643          W 19981214 <--

OTHER SOURCE(S):          MARPAT 131:44844
ED   Entered STN:   01 Jul 1999
GI

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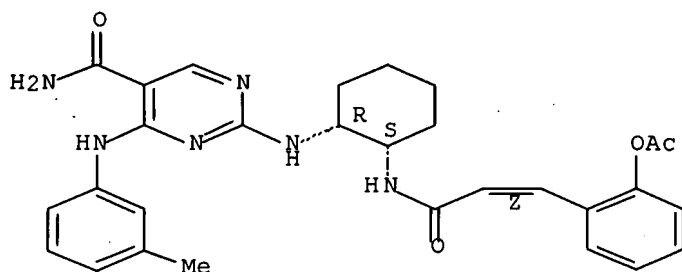
AB Pyrimidine-5-carboxamide derivs. or salts [I; X = O, S, NR1, CO, NR1CO, CONR1, C=NOR1, a bond; Y = lower alkylene optionally substituted by OR1 or NHR1, a bond; Z = O, NR2, a bond; A = H, optionally substituted lower alkyl, lower alkyl optionally having CO, optionally substituted aryl or heteroaryl, optionally substituted cycloalkyl, optionally substituted and saturated N heterocycle; B = optionally substituted aryl or heteroaryl; R1, R2 = H or lower alkyl optionally containing CO], effective tyrosinase inhibitors useful as 5-HT antagonists, antiallergics, were prepared I showed IC50 < 0.1 μ M in scintillation proximity assay. I were effective at 0.1-10 mg/kg-day p.o.

IT 227449-98-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel pyrimidine-5-carboxamide derivs. as tyrosinase inhibitors)

RN 227449-98-1 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[[(1R,2S)-2-[[[(2Z)-3-[2-(acetyloxy)phenyl]-1-oxo-2-propenyl]amino]cyclohexyl]amino]-4-[(3-methylphenyl)amino]-, rel-(9CI) (CA INDEX NAME)

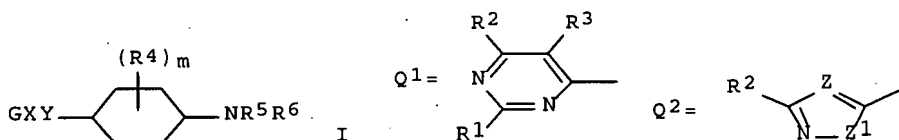
Relative stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 26 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1999:404940 CAPLUS Full-text
 DOCUMENT NUMBER: 131:44606
 TITLE: Preparation of cyclohexylamine derivatives as arthropodocides and fungicides
 INVENTOR(S): Lee, Kevin Chun
 PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
 SOURCE: PCT Int. Appl., 115 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------------|
| WO 9931072 | A1 | 19990624 | WO 1998-US26013 | 19981208 <-- |
| W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU | | | | |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| IN 1997CA01507 | A | 20050311 | IN 1997-CA1507 | 19970814 <-- |
| AU 9916316 | A | 19990705 | AU 1999-16316 | 19981208 <-- |
| PRIORITY APPLN. INFO.: | | | US 1997-69994P | P 19971218 <-- |
| | | | WO 1998-US26013 | W 19981208 <-- |
| OTHER SOURCE(S): MARPAT 131:44606 | | | | |
| ED Entered STN: 01 Jul 1999 | | | | |
| GI | | | | |



AB The title compds. I [G = Q1, Q2; Y is a direct bond or C1-C4 alkylene optionally substituted with C1-C4 alkyl; X is O, NR7 or S(O)p; each Z is independently selected from N and CR3; each Z1 is independently selected from O, S and NR8; and R1-R8, m and p are as defined in the disclosure], arthropodocides and fungicides, were prepared E.g., cis-N-N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-1,4-cyclohexanediamine was prepared The activity of I against fall armyworm, two-spotted spider mite, Erysiphe graminis, etc., was determined

IT 227469-23-0P 227469-37-6P 227469-68-3P

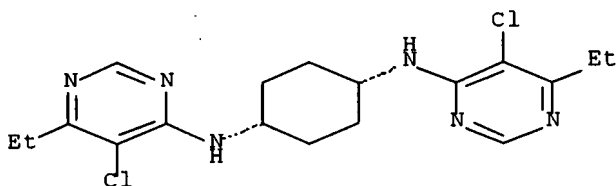
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of cyclohexylamine derivs. as arthropodocides and fungicides)

RN 227469-23-0 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-, cis- (9CI) (CA INDEX NAME)

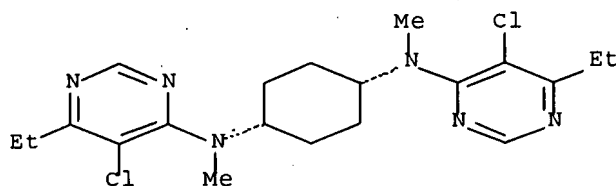
Relative stereochemistry.



RN 227469-37-6 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N,N'-dimethyl-, cis- (9CI) (CA INDEX NAME)

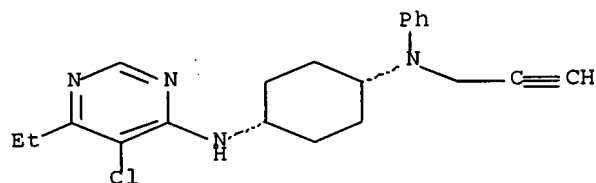
Relative stereochemistry.



RN 227469-68-3 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-phenyl-N-2-propynyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



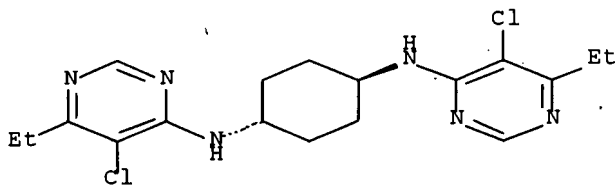
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 227469-92-3P 227469-93-4P 227469-94-5P
 227469-95-6P 227470-15-7P 227470-16-8P
 227470-17-9P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of cyclohexylamine derivs. as arthropodicides and fungicides)

RN 227469-24-1 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-, trans- (9CI) (CA INDEX NAME)

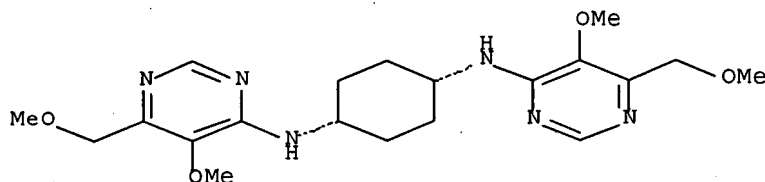
Relative stereochemistry.



RN 227469-27-4 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis[5-methoxy-6-(methoxymethyl)-4-pyrimidinyl]-, cis- (9CI) (CA INDEX NAME)

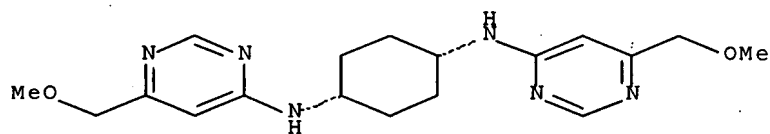
Relative stereochemistry.



RN 227469-28-5 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis[6-(methoxymethyl)-4-pyrimidinyl]-, cis- (9CI) (CA INDEX NAME)

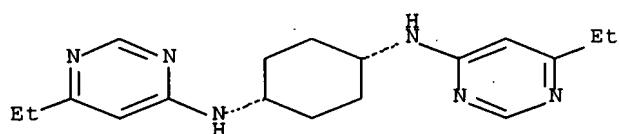
Relative stereochemistry.



RN 227469-30-9 CAPLUS

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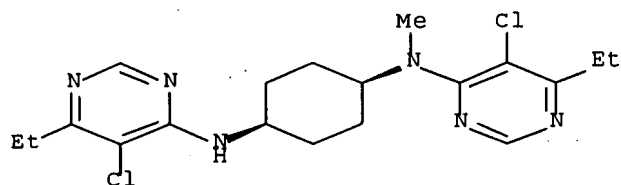
Relative stereochemistry.



RN 227469-32-1 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-, cis- (9CI) (CA INDEX NAME)

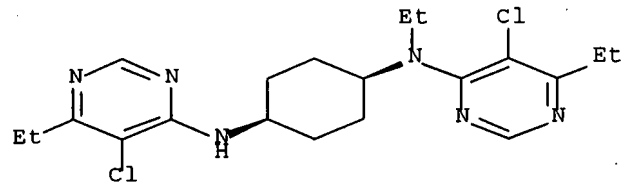
Relative stereochemistry.



RN 227469-33-2 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N-ethyl-, cis- (9CI) (CA INDEX NAME)

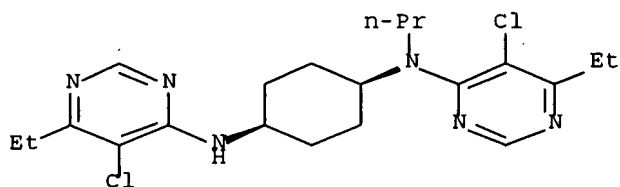
Relative stereochemistry.



RN 227469-34-3 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N-propyl-, cis- (9CI) (CA INDEX NAME)

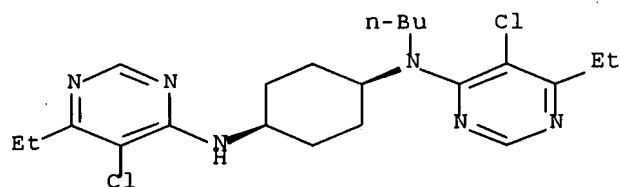
Relative stereochemistry.



RN 227469-35-4 CAPLUS

CN 1,4-Cyclohexanediamine, N-butyl-N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-, cis- (9CI) (CA INDEX NAME)

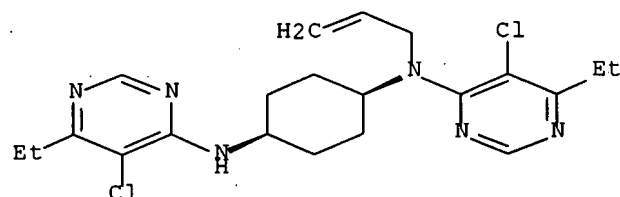
Relative stereochemistry.



RN 227469-36-5 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N-2-propenyl-, cis- (9CI) (CA INDEX NAME)

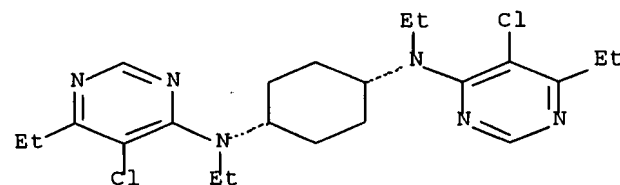
Relative stereochemistry.



RN 227469-38-7 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N,N'-diethyl-, cis- (9CI) (CA INDEX NAME)

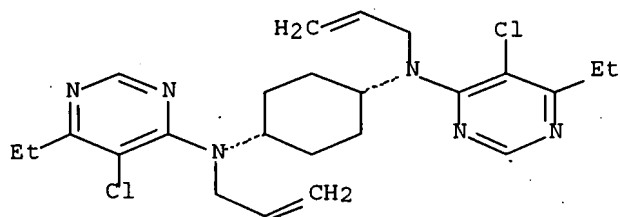
Relative stereochemistry.



RN 227469-39-8 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N,N'-di-2-propenyl-, cis- (9CI) (CA INDEX NAME)

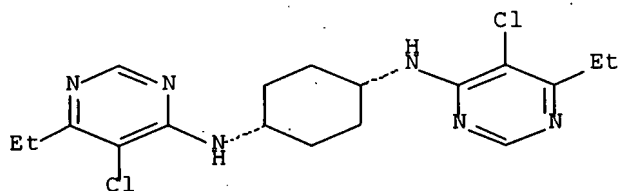
Relative stereochemistry.



RN 227469-40-1 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-, dihydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

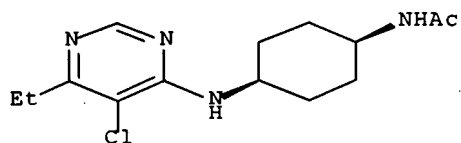


●2 HCl

RN 227469-41-2 CAPLUS

CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]- (9CI) (CA INDEX NAME)

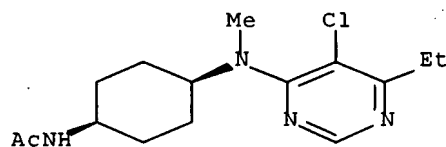
Relative stereochemistry.



RN 227469-42-3 CAPLUS

CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)methylamino]cyclohexyl]- (9CI) (CA INDEX NAME)

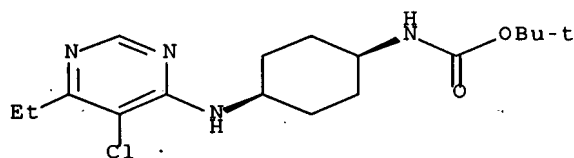
Relative stereochemistry.



RN 227469-43-4 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

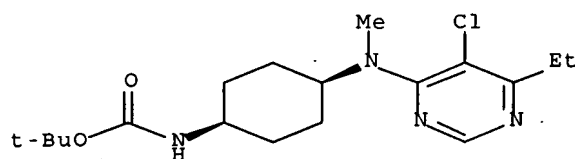
Relative stereochemistry.



RN 227469-44-5 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)methylamino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

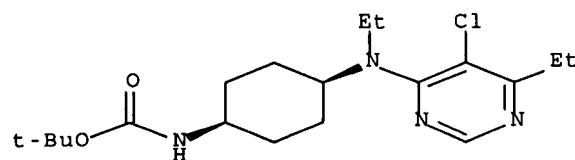
Relative stereochemistry.



RN 227469-45-6 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)ethylamino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

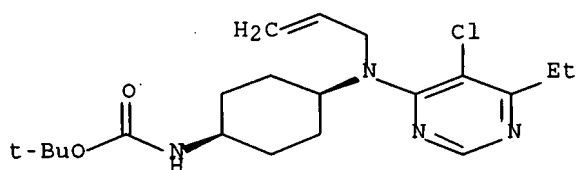
Relative stereochemistry.



RN 227469-46-7 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)-2-propenylamino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

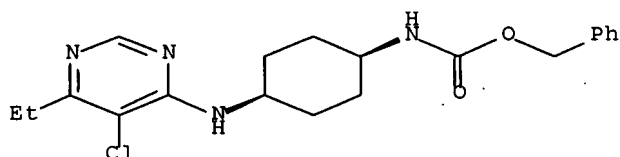
Relative stereochemistry.



RN 227469-47-8 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

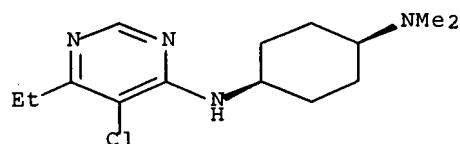
Relative stereochemistry.



RN 227469-53-6 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N,N-dimethyl-, cis- (9CI) (CA INDEX NAME)

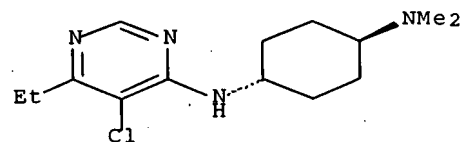
Relative stereochemistry.



RN 227469-54-7 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N,N-dimethyl-, trans- (9CI) (CA INDEX NAME)

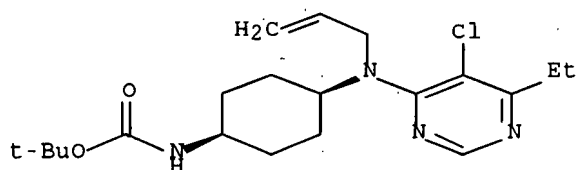
Relative stereochemistry.



RN 227469-55-8 CAPLUS

CN 1,4-Cyclohexanediamine, N-butyl-N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-, cis- (9CI) (CA INDEX NAME)

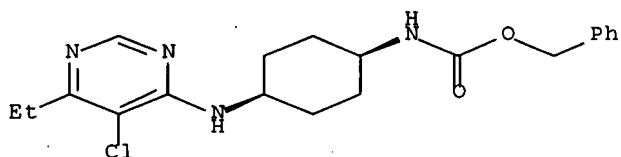
Relative stereochemistry.



RN 227469-47-8 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

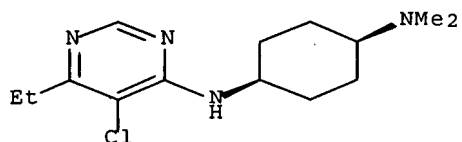
Relative stereochemistry.



RN 227469-53-6 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N,N-dimethyl-, cis- (9CI) (CA INDEX NAME)

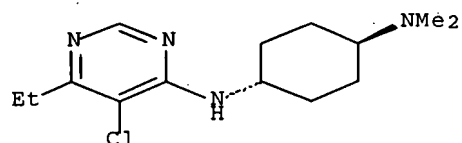
Relative stereochemistry.



RN 227469-54-7 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N,N-dimethyl-, trans- (9CI) (CA INDEX NAME)

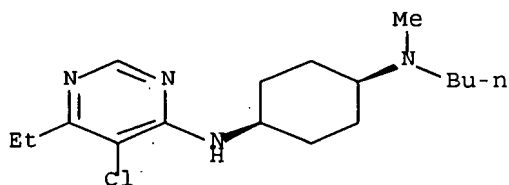
Relative stereochemistry.



RN 227469-55-8 CAPLUS

CN 1,4-Cyclohexanediamine, N-butyl-N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-, cis- (9CI) (CA INDEX NAME)

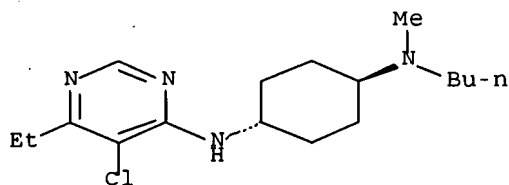
Relative stereochemistry.



RN 227469-56-9 CAPLUS

CN 1,4-Cyclohexanediamine, N-butyl-N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-, trans- (9CI) (CA INDEX NAME)

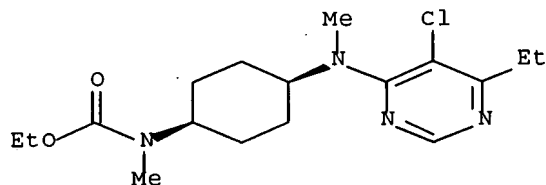
Relative stereochemistry.



RN 227469-57-0 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)methylamino]cyclohexyl]methyl-, ethyl ester (9CI) (CA INDEX NAME)

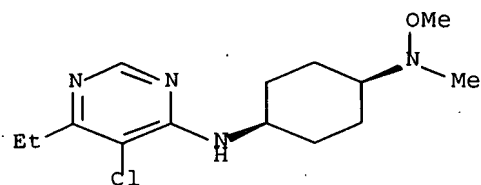
Relative stereochemistry.



RN 227469-58-1 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methoxy-N-methyl-, cis- (9CI) (CA INDEX NAME)

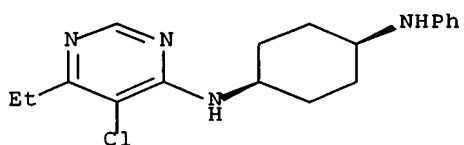
Relative stereochemistry.



RN 227469-59-2 CAPLUS

CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-phenyl-, cis- (9CI) (CA INDEX NAME)

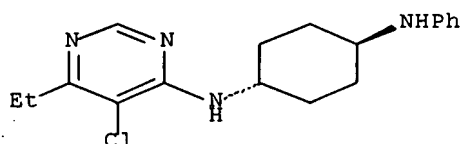
Relative stereochemistry.



RN 227469-60-5 CAPLUS

CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-phenyl-, trans- (9CI) (CA INDEX NAME)

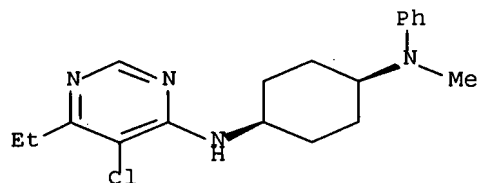
Relative stereochemistry.



RN 227469-61-6 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-N-phenyl-, cis- (9CI) (CA INDEX NAME)

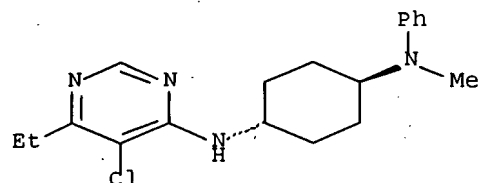
Relative stereochemistry.



RN 227469-62-7 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-N-phenyl-, trans- (9CI) (CA INDEX NAME)

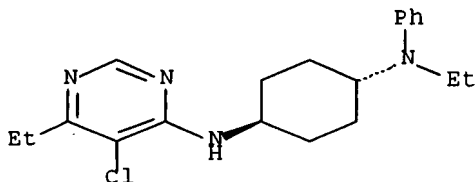
Relative stereochemistry.



RN 227469-63-8 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-ethyl-N-phenyl-, trans- (9CI) (CA INDEX NAME)

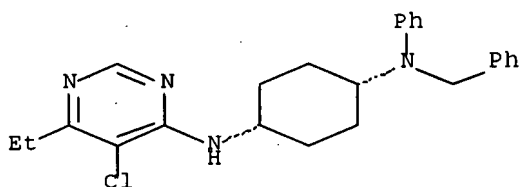
Relative stereochemistry.



RN 227469-64-9 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-phenyl-N-(phenylmethyl)-, cis- (9CI) (CA INDEX NAME)

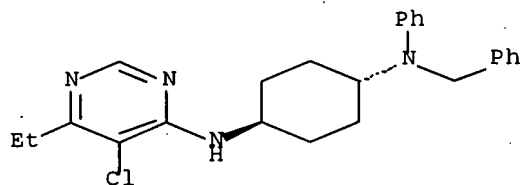
Relative stereochemistry.



RN 227469-65-0 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-phenyl-N-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

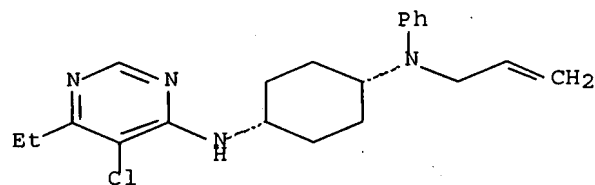
Relative stereochemistry.



RN 227469-66-1 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-phenyl-N-2-propenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

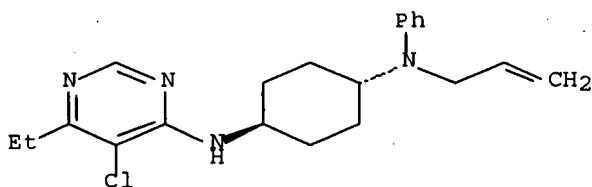


RN 227469-67-2 CAPLUS

CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-phenyl-N-2-

propenyl-, trans- (9CI) (CA INDEX NAME)

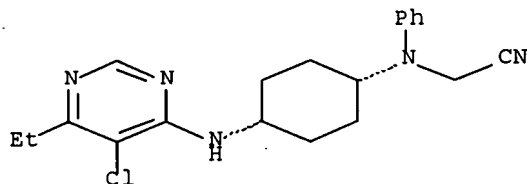
Relative stereochemistry.



RN 227469-69-4 CAPLUS

CN Acetonitrile, [[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenylamino]- (9CI) (CA INDEX NAME)

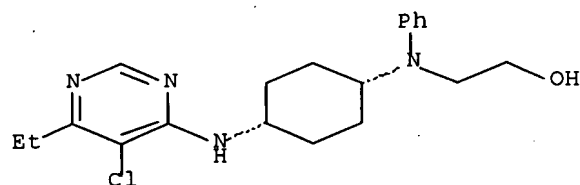
Relative stereochemistry.



RN 227469-70-7 CAPLUS

CN Ethanol, 2-[[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenylamino]- (9CI) (CA INDEX NAME)

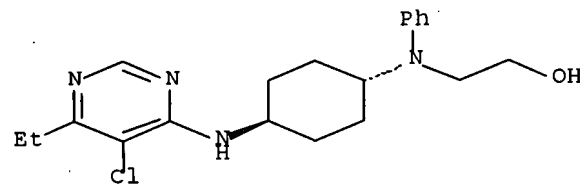
Relative stereochemistry.



RN 227469-71-8 CAPLUS

CN Ethanol, 2-[[trans-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenylamino]- (9CI) (CA INDEX NAME)

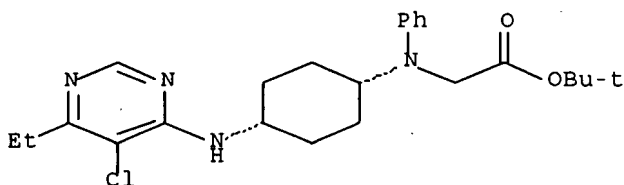
Relative stereochemistry.



RN 227469-72-9 CAPLUS

CN Glycine, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

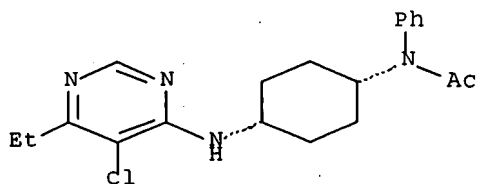
Relative stereochemistry.



RN 227469-73-0 CAPLUS

CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl- (9CI) (CA INDEX NAME)

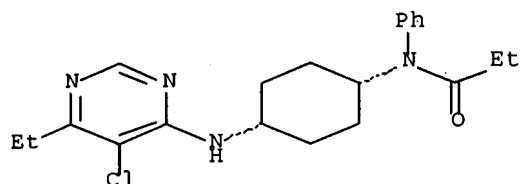
Relative stereochemistry.



RN 227469-74-1 CAPLUS

CN Propanamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl- (9CI) (CA INDEX NAME)

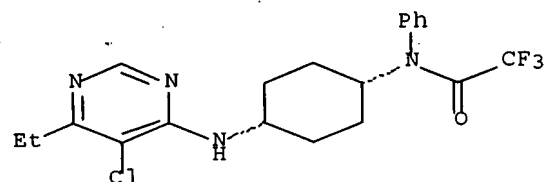
Relative stereochemistry.



RN 227469-75-2 CAPLUS

CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-2,2,2-trifluoro-N-phenyl- (9CI) (CA INDEX NAME)

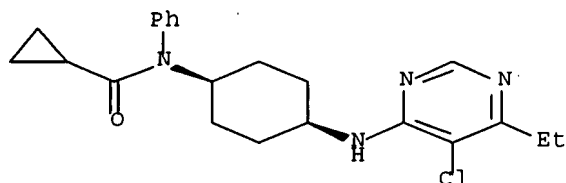
Relative stereochemistry.



RN 227469-76-3 CAPLUS

CN Cyclopropanecarboxamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl- (9CI) (CA INDEX NAME)

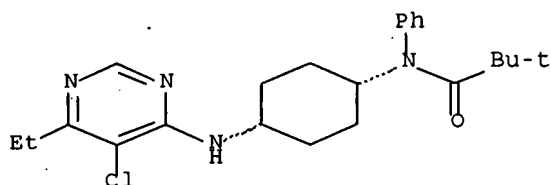
Relative stereochemistry.



RN 227469-77-4 CAPLUS

CN Propanamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-2,2-dimethyl-N-phenyl- (9CI) (CA INDEX NAME)

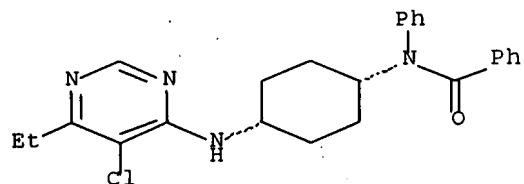
Relative stereochemistry.



RN 227469-78-5 CAPLUS

CN Benzamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl- (9CI) (CA INDEX NAME)

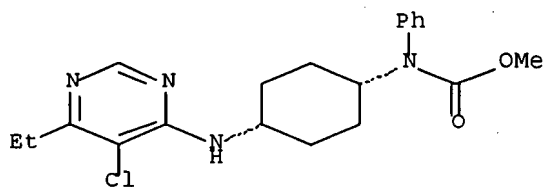
Relative stereochemistry.



RN 227469-79-6 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, methyl ester (9CI) (CA INDEX NAME)

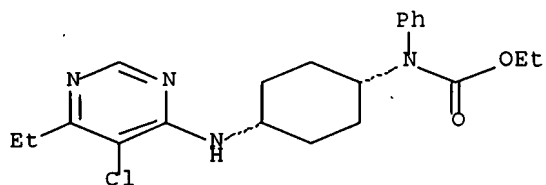
Relative stereochemistry.



RN 227469-80-9 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, ethyl ester (9CI) (CA INDEX NAME)

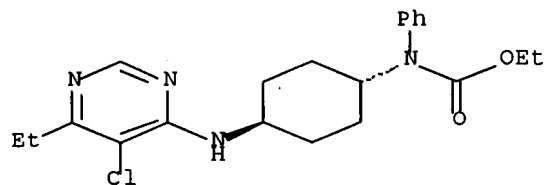
Relative stereochemistry.



RN 227469-81-0 CAPLUS

CN Carbamic acid, [trans-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, ethyl ester (9CI) (CA INDEX NAME)

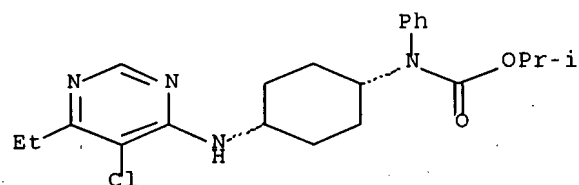
Relative stereochemistry.



RN 227469-82-1 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)

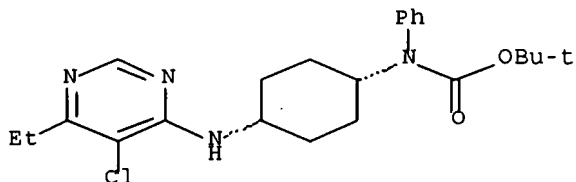
Relative stereochemistry.



RN 227469-83-2 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

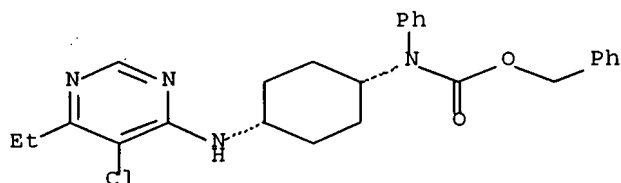
Relative stereochemistry.



RN 227469-84-3 CAPLUS

CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

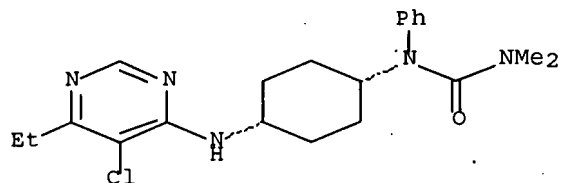
Relative stereochemistry.



RN 227469-85-4 CAPLUS

CN Urea, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N',N'-dimethyl-N-phenyl- (9CI) (CA INDEX NAME)

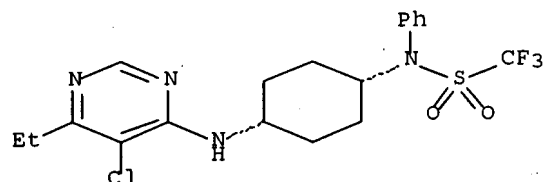
Relative stereochemistry.



RN 227469-86-5 CAPLUS

CN Methanesulfonamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-1,1,1-trifluoro-N-phenyl- (9CI) (CA INDEX NAME)

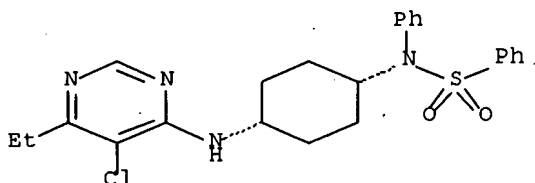
Relative stereochemistry.



RN 227469-87-6 CAPLUS

CN Benzenesulfonamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl- (9CI) (CA INDEX NAME)

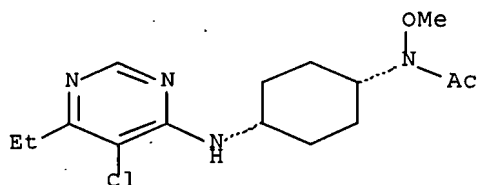
Relative stereochemistry.



RN 227469-88-7 CAPLUS

CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-methoxy- (9CI) (CA INDEX NAME)

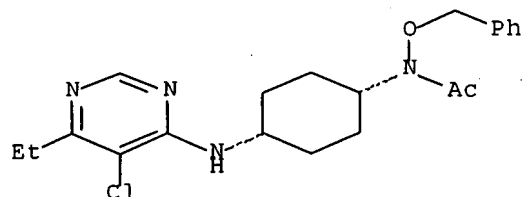
Relative stereochemistry.



RN 227469-89-8 CAPLUS

CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-(phenylmethoxy)- (9CI) (CA INDEX NAME)

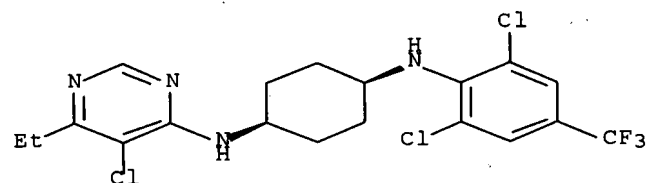
Relative stereochemistry.



RN 227469-90-1 CAPLUS

CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-[2,6-dichloro-4-(trifluoromethyl)phenyl]-, cis- (9CI) (CA INDEX NAME)

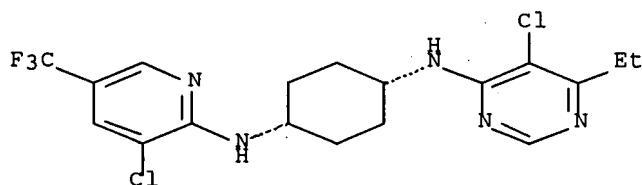
Relative stereochemistry.



RN 227469-91-2 CAPLUS

CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-, cis- (9CI) (CA INDEX NAME)

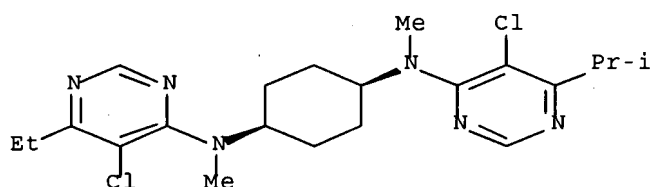
Relative stereochemistry.



RN 227469-92-3 CAPLUS

CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-[5-chloro-6-(1-methylethyl)-4-pyrimidinyl]-N,N'-dimethyl-, cis- (9CI) (CA INDEX NAME)

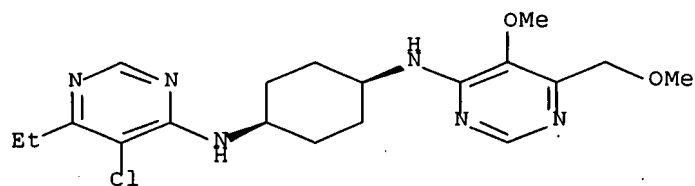
Relative stereochemistry.



RN 227469-93-4 CAPLUS

CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-[5-methoxy-6-(methoxymethyl)-4-pyrimidinyl]-, cis- (9CI) (CA INDEX NAME)

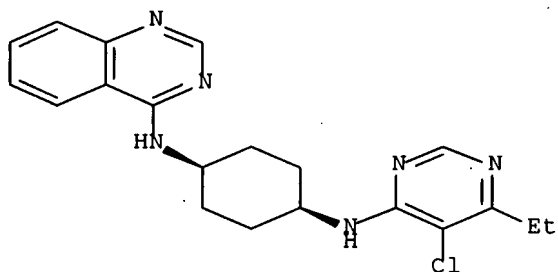
Relative stereochemistry.



RN 227469-94-5 CAPLUS

CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-4-quinazolinyl-, cis- (9CI) (CA INDEX NAME)

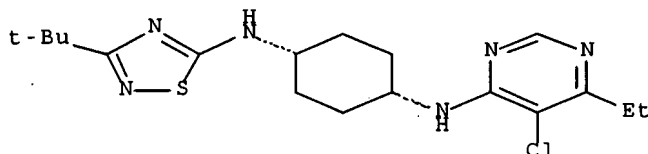
Relative stereochemistry.



RN 227469-95-6 CAPLUS

CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-[3-(1,1-dimethylethyl)-1,2,4-thiadiazol-5-yl]-, cis- (9CI) (CA INDEX NAME)

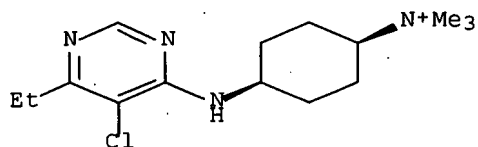
Relative stereochemistry.



RN 227470-15-7 CAPLUS

CN Cyclohexanaminium, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-N,N,N-trimethyl-, iodide, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

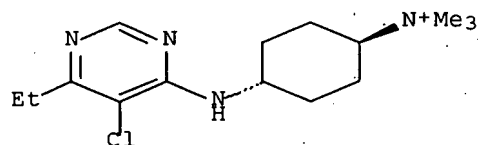


● I⁻

RN 227470-16-8 CAPLUS

CN Cyclohexanaminium, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-N,N,N-trimethyl-, iodide, trans- (9CI) (CA INDEX NAME)

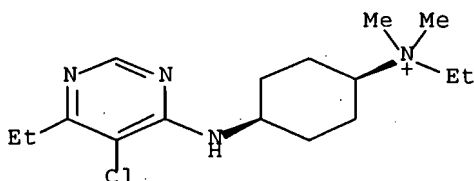
Relative stereochemistry.



● I⁻

RN 227470-17-9 CAPLUS
 CN Cyclohexanaminium, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-N-ethyl-N,N-dimethyl-, iodide, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 27 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:85304 CAPLUS Full-text

DOCUMENT NUMBER: 128:212665

TITLE: Aminopyrimidines with High Affinity for Both Serotonin and Dopamine Receptors

AUTHOR(S): Wustrow, David; Belliotti, Thomas; Glase, Shelly; Kesten, Suzanne Ross; Johnson, Don; Colbry, Norman; Rubin, Ronald; Blackburn, Anthony; Akunne, Hyacinth; Corbin, Ann; Davis, M. Duff; Georgic, Lynn; Whetzel, Steven; Zoski, Kim; Heffner, Thomas; Pugsley, Thomas; Wise, Lawrence

CORPORATE SOURCE: Departments of Chemistry Chemical Development and Therapeutics, Parke-Davis Pharmaceutical Research Division of Warner-Lambert Company, Ann Arbor, MI, 48105, USA

SOURCE: Journal of Medicinal Chemistry (1998), 41(5), 760-771

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 14 Feb 1998

AB A series of {4-[2-(4-arylpiperazin-1-yl)alkyl]cyclohexyl}pyrimidin-2-ylamines were prepared and found to have receptor binding affinity for D2 and D3 dopamine (DA) receptors and serotonin 5-HT1A receptors. The structural contributions to D2/D3 and 5-HT1A receptor binding of the aminopyrimidine, cycloalkyl, and phenylpiperazine portions of the mol. were examined. Compds. having potent affinity for both DA D2 and 5-HT1A receptors were evaluated for intrinsic activity at these receptors, in vitro and in vivo. One of the compds. (PD 158771) had a profile indicative of partial agonist activity at both D2 and 5-HT1A receptors causing partially decreased synthesis of the neurotransmitters DA and 5-HT and their metabolites. This compound has a profile in behavioral tests that is predictive of antipsychotic activity, suggesting that mixed partial agonists may have utility as antipsychotic agents with increased efficacy and decreased side effects.

IT 204245-70-5P 204245-89-6P

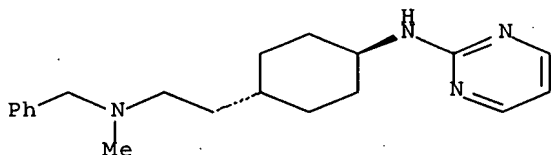
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of aminopyrimidines with affinity for serotonin and dopamine receptors)

RN 204245-70-5 CAPLUS

CN 2-Pyrimidinamine, N-[4-[2-[methyl(phenylmethyl)amino]ethyl]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

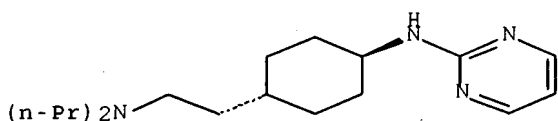
Relative stereochemistry.



RN 204245-89-6 CAPLUS

CN 2-Pyrimidinamine, N-[4-[2-(dipropylamino)ethyl]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 189153-07-9P

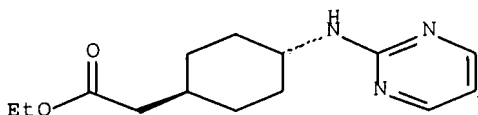
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminopyrimidines with affinity for serotonin and dopamine receptors)

RN 189153-07-9 CAPLUS

CN Cyclohexanecarboxylic acid, 4-(2-pyrimidinylamino)-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

43

THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 28 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:321401 CAPLUS Full-text

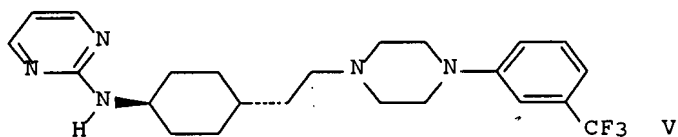
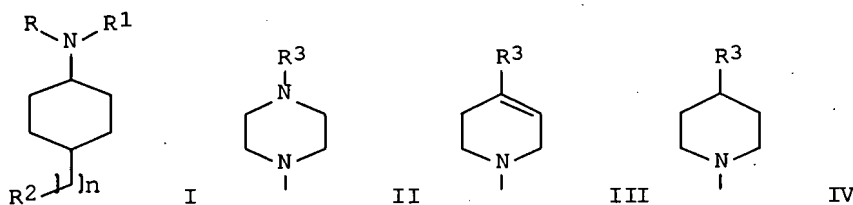
DOCUMENT NUMBER: 126:293365

TITLE: Preparation of heteroaryl-substituted cyclohexylamines as central nervous system (CNS) agents

INVENTOR(S): Belliotti, Thomas R.; Kesten, Suzanne R.; Pugsley,

Thomas A.; Wustrow, David J.
 PATENT ASSIGNEE(S): Warner-Lambert Company, USA
 SOURCE: PCT Int. Appl., 61 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|-------------------|-----------------|----------------|
| WO 9711070 | A1 | 19970327 | WO 1996-US13687 | 19960823 <-- |
| W: AU, BG, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KR, LK, LR, LT, LV, MG, MX, NO, NZ, PL, RO, SG, SI, SK, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9668590 | A | 19970409 | AU 1996-68590 | 19960823 <-- |
| ZA 9607944 | A | 19970402 | ZA 1996-7944 | 19960919 <-- |
| US 5977110 | A | 19991102 | US 1998-43331 | 19980320 <-- |
| PRIORITY APPLN. INFO.: | | | US 1995-4193P | P 19950922 <-- |
| | | | WO 1996-US13687 | W 19960823 <-- |
| OTHER SOURCE(S): | | MARPAT 126:293365 | | |
| ED Entered STN: | | 21 May 1997 | | |
| GI | | | | |



AB The title compds. [I; R = heteroaryl; R1 = H, lower alkyl, cycloalkyl, aryl, PhCH2; n = 1-2; R2 = II, III, IV (wherein R3 = (un)substituted 2-pyrimidinyl, 2-, 3- or 4-pyridinyl, 2- or 3-thienyl, etc.)], useful as CNS agents, and particularly useful as dopaminergic, serotonergic, antipsychotic, and anxiolytic agents, and for treatment of schizophrenia, were prepared Thus, reaction of trans-(4-aminocyclohexyl)acetic acid Et ester with 2-chloropyrimidine in the presence of Et3N in EtOH followed by reduction of the resulting trans-[4-(pyrimidin-2-ylamino)cyclohexyl]acetic acid Et ester with LiAlH4 in THF, treatment of trans-[4-(pyrimidin-2-ylamino)cyclohexyl]ethanol with CBr4 in the presence of polymer-supported Ph3P in CH2Cl2, and reaction of trans-[4-(2-bromoethyl)cyclohexyl]pyrimidin-2-ylamine with 1-(3-

trifluoromethylphenyl)piperazine in the presence of K₂CO₃ in MeCN afforded trans-V which showed K_i of 6 nM against [3H]N-0437 binding to h-D₂ receptors.

IT 189153-07-9P

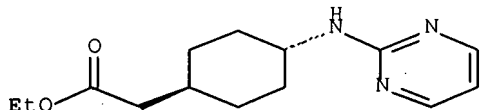
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted cyclohexylamines as central nervous system (CNS) agents)

RN 189153-07-9 CAPLUS

CN Cyclohexaneacetic acid, 4-(2-pyrimidinylamino)-, ethyl ester, trans- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



L23 ANSWER 29 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:391643 CAPLUS' Full-text

DOCUMENT NUMBER: 125:58537

TITLE: Preparation of 4-cyclohexylaminopyrimidine derivatives for agrohorticultural pest control

INVENTOR(S): Obata, Tokio; Fujii, Katsutoshi; Tsutsumiuchi, Kiyoshi; Yamanaka, Yoshinori

PATENT ASSIGNEE(S): Japan

SOURCE: PCT Int. Appl., 83 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

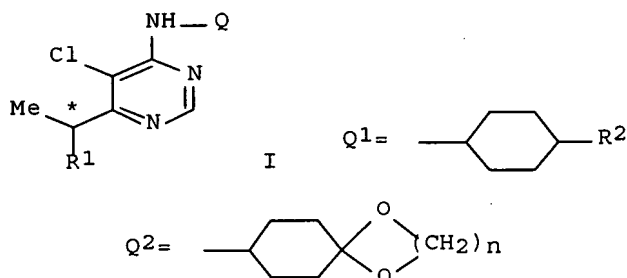
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| WO 9606086 | A1 | 19960229 | WO 1995-JP1665 | 19950823 <-- |
| W: KR, US | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| JP 08113564 | A | 19960507 | JP 1995-213416 | 19950822 <-- |
| JP 3211636 | B2 | 20010925 | | |

PRIORITY APPLN. INFO.: JP 1994-198262 A 19940823 <--

OTHER SOURCE(S): MARPAT 125:58537

ED Entered STN: 09 Jul 1996

GI



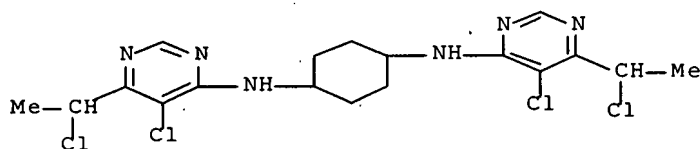
AB The title compds. (I; R1 = halo, C2-5 acyloxy, hydroxy, C1-4 alkoxy, C1-4 alkylthio; Q = Q1, Q2; wherein R2 = C1-8 alkyl, Ph, pyrimidinylamino, C1-6 alkoxy, CO2R3, amino, NHCOR4; wherein R3 = C1-4 alkyl, H; R4 = C1-8 alkyl or alkoxy; the asterisked C atom represents an asym. C atom), useful as insecticides, acaricides, and fungicides, are prepared Thus, a mixture of cis- and trans-4-tert-butylcyclohexylamine (3 g) was dissolved in PhMe, treated with 6.3 g 4,5-dichloro-6-(1-chloroethyl)pyrimidine, and heated with stirring at .apprx.60° for 4 h to give 1.3 g cis-I (R1 = Cl, Q = Q1, R2 = tert-butyl) (II) and 0.9 g trans-I (R1 = Cl, Q = Q1, R2 = tert-butyl). Rice seedlings, which were dipped in a 300 ppm solution of the cis-isomer II and dried, killed 100% Nephrotettix cincticeps larvae.

IT 178202-34-1P 178202-35-2P 178202-36-3P
 178202-37-4P 178202-38-5P 178202-39-6P
 178202-40-9P 178202-61-4P 178202-62-5P
 178202-63-6P 178202-64-7P 178202-65-8P
 178202-67-0P 178202-68-1P 178202-69-2P
 178202-70-5P 178202-71-6P 178202-72-7P
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 178203-22-0P 178203-23-1P 178203-24-2P
 178203-25-3P 178203-26-4P 178203-27-5P
 178203-28-6P 178203-29-7P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of (cyclohexylamino)pyrimidine derivs. for agrohorticultural pest control)

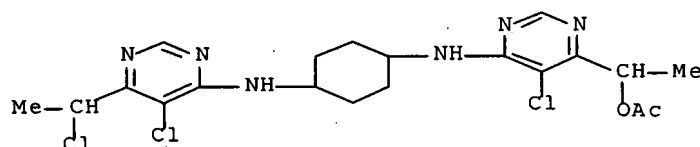
RN 178202-34-1 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]-
 (9CI) (CA INDEX NAME)

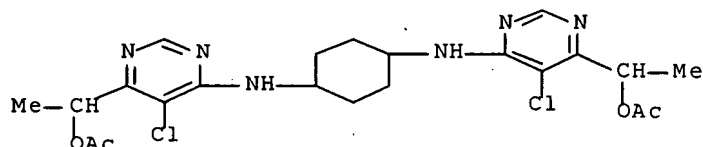


RN 178202-35-2 CAPLUS

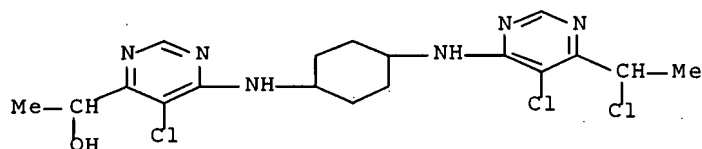
CN 4-Pyrimidinemethanol, 5-chloro-6-[[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]amino]-α-methyl-, acetate (ester) (9CI)
 (CA INDEX NAME)



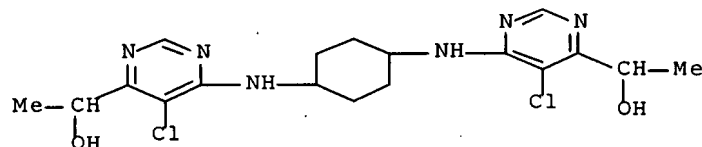
RN 178202-36-3 CAPLUS

CN 4-Pyrimidinemethanol, 5,5'-(1,4-cyclohexanediylldiimino)bis[5-chloro- α -methyl-, diacetate (ester) (9CI) (CA INDEX NAME)

RN 178202-37-4 CAPLUS

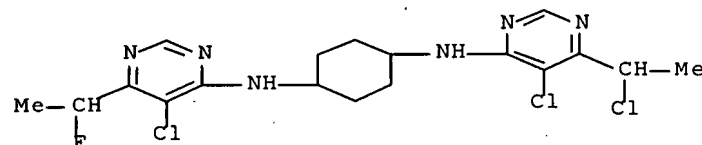
CN 4-Pyrimidinemethanol, 5-chloro-6-[[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]amino]- α -methyl- (9CI) (CA INDEX NAME)

RN 178202-38-5 CAPLUS

CN 4-Pyrimidinemethanol, 5,5'-(1,4-cyclohexanediylldiimino)bis[5-chloro- α -methyl- (9CI) (CA INDEX NAME)

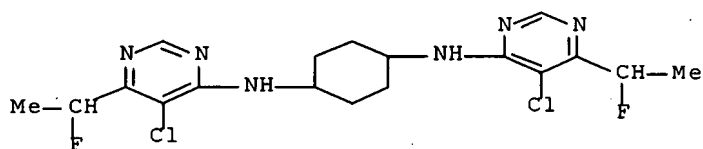
RN 178202-39-6 CAPLUS

CN 1,4-Cyclohexanediamine, N-[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]-N'-[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 178202-40-9 CAPLUS

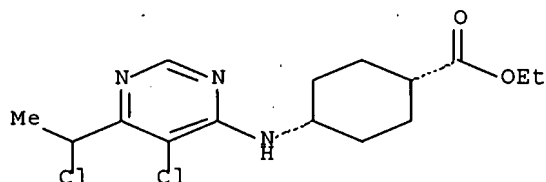
CN 1,4-Cyclohexanediamine, N,N'-bis[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 178202-61-4 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

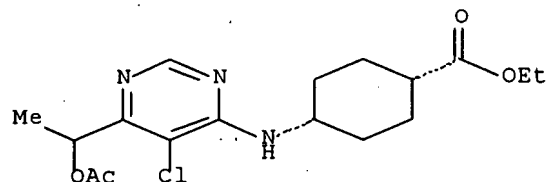
Relative stereochemistry.



RN 178202-62-5 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

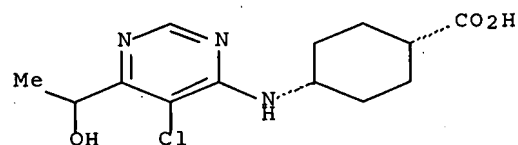
Relative stereochemistry.



RN 178202-63-6 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]-, cis- (9CI) (CA INDEX NAME)

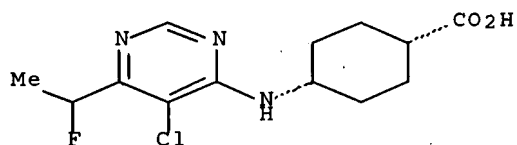
Relative stereochemistry.



RN 178202-64-7 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]-, cis- (9CI) (CA INDEX NAME)

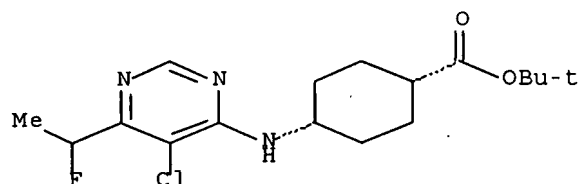
Relative stereochemistry.



RN 178202-65-8 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

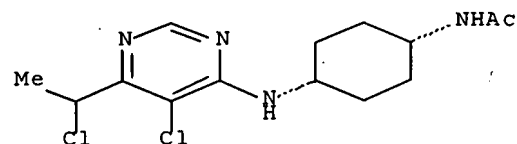
Relative stereochemistry.



RN 178202-67-0 CAPLUS

CN Acetamide, N-[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, cis- (9CI) (CA INDEX NAME)

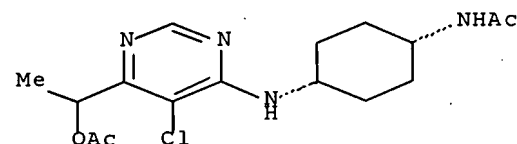
Relative stereochemistry.



RN 178202-68-1 CAPLUS

CN Acetamide, N-[4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-, cis- (9CI) (CA INDEX NAME)

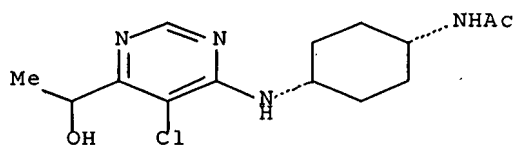
Relative stereochemistry.



RN 178202-69-2 CAPLUS

CN Acetamide, N-[4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-, cis- (9CI) (CA INDEX NAME)

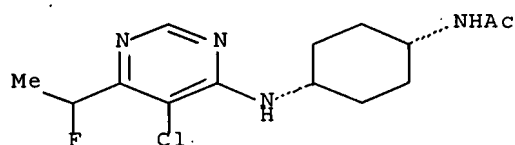
Relative stereochemistry.



RN 178202-70-5 CAPLUS

CN Acetamide, N-[4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, cis- (9CI) (CA INDEX NAME)

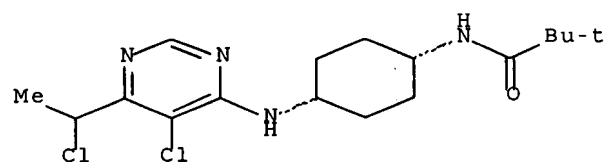
Relative stereochemistry.



RN 178202-71-6 CAPLUS

CN Propanamide, N-[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, cis- (9CI) (CA INDEX NAME)

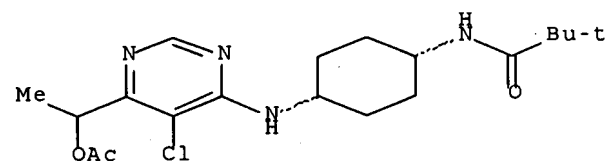
Relative stereochemistry.



RN 178202-72-7 CAPLUS

CN Propanamide, N-[4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, cis- (9CI) (CA INDEX NAME)

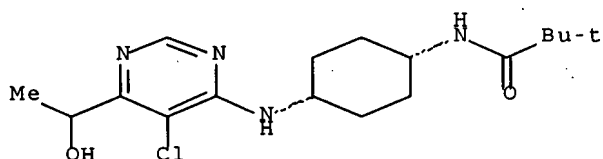
Relative stereochemistry.



RN 178202-73-8 CAPLUS

CN Propanamide, N-[4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, cis- (9CI) (CA INDEX NAME)

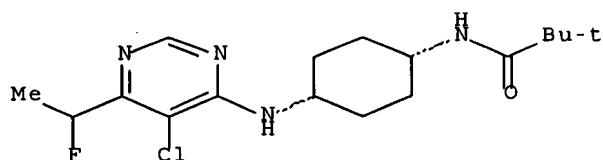
Relative stereochemistry.



RN 178202-74-9 CAPLUS

CN Propanamide, N-[4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, cis- (9CI) (CA INDEX NAME)

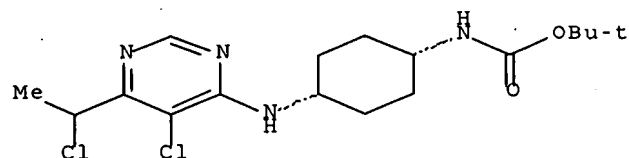
Relative stereochemistry.



RN 178202-75-0 CAPLUS

CN Carbamic acid, [4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

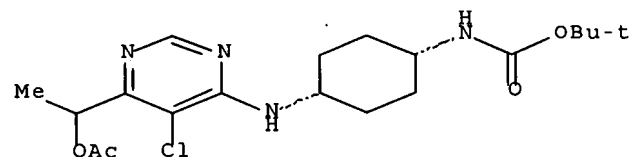
Relative stereochemistry.



RN 178202-76-1 CAPLUS

CN Carbamic acid, [4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

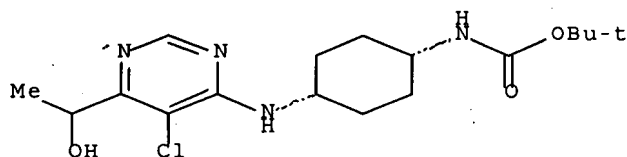
Relative stereochemistry.



RN 178202-77-2 CAPLUS

CN Carbamic acid, [4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

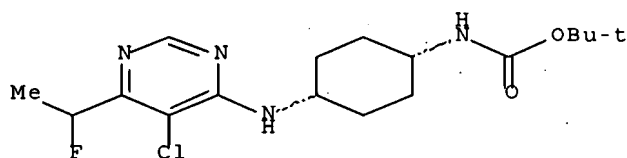
Relative stereochemistry.



RN 178202-78-3 CAPLUS

CN Carbamic acid, [4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

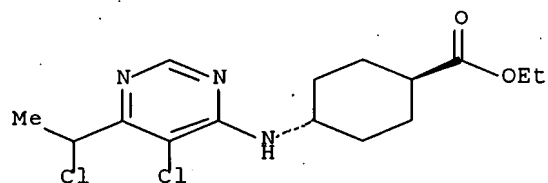
Relative stereochemistry.



RN 178203-12-8 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]-, ethyl ester, trans- (9CI) (CA INDEX NAME)

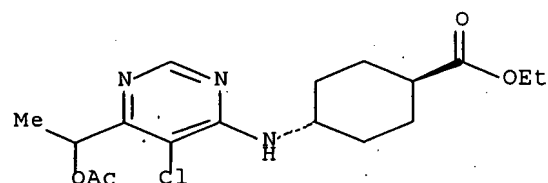
Relative stereochemistry.



RN 178203-13-9 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]-, ethyl ester, trans- (9CI) (CA INDEX NAME)

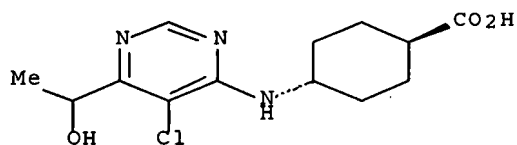
Relative stereochemistry.



RN 178203-14-0 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

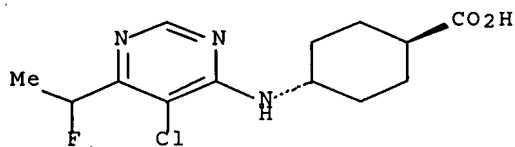
Relative stereochemistry.



RN 178203-15-1 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

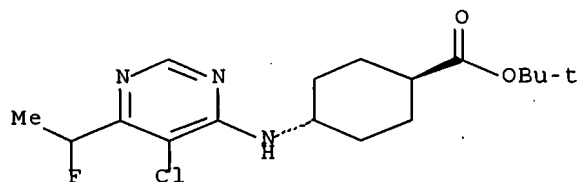
Relative stereochemistry.



RN 178203-16-2 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

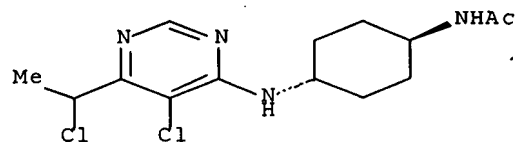
Relative stereochemistry.



RN 178203-18-4 CAPLUS

CN Acetamide, N-[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

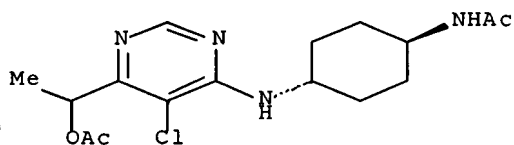
Relative stereochemistry.



RN 178203-19-5 CAPLUS

CN Acetamide, N-[4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

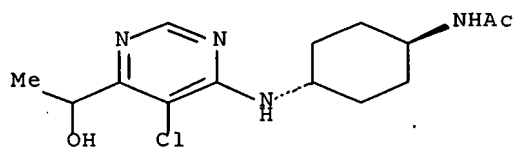
Relative stereochemistry.



RN 178203-20-8 CAPLUS

CN Acetamide, N-[4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

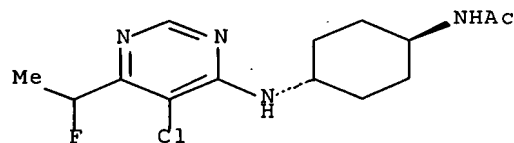
Relative stereochemistry.



RN 178203-21-9 CAPLUS

CN Acetamide, N-[4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

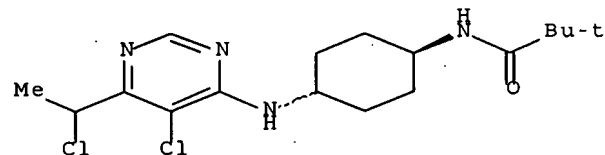
Relative stereochemistry.



RN 178203-22-0 CAPLUS

CN Propanamide, N-[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, trans- (9CI) (CA INDEX NAME)

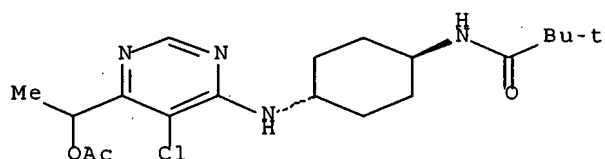
Relative stereochemistry.



RN 178203-23-1 CAPLUS

CN Propanamide, N-[4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, trans- (9CI) (CA INDEX NAME)

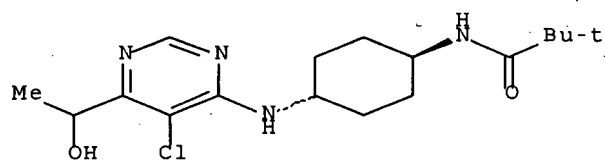
Relative stereochemistry.



RN 178203-24-2 CAPLUS

CN Propanamide, N-[4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, trans- (9CI) (CA INDEX NAME)

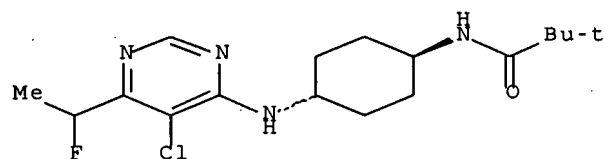
Relative stereochemistry.



RN 178203-25-3 CAPLUS

CN Propanamide, N-[4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, trans- (9CI) (CA INDEX NAME)

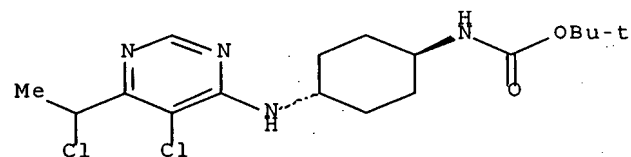
Relative stereochemistry.



RN 178203-26-4 CAPLUS

CN Carbamic acid, [4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

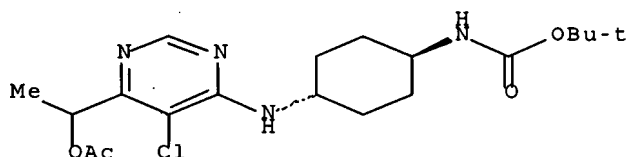
Relative stereochemistry.



RN 178203-27-5 CAPLUS

CN Carbamic acid, [4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

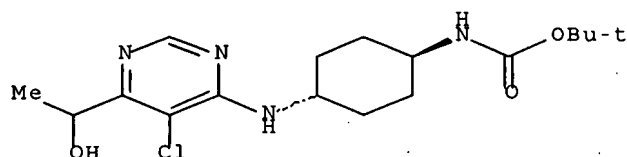
Relative stereochemistry.



RN 178203-28-6 CAPLUS

CN Carbamic acid, [4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

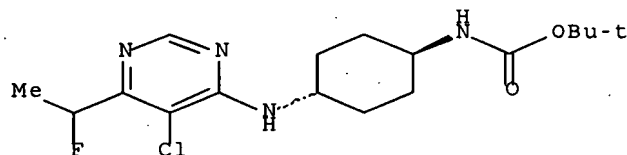
Relative stereochemistry.



RN 178203-29-7 CAPLUS

CN Carbamic acid, [4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L23 ANSWER 30 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:369682 CAPLUS Full-text

DOCUMENT NUMBER: 125:33666

TITLE: Preparation of 4-(cycloalkylamino)pyrimidines and analogs as pesticides and agrochemical fungicides

INVENTOR(S): Maerkl, Martin; Schaper, Wolfgang; Knauf, Werner; Sanft, Ulrich; Kern, Manfred; Bonin, Werner; Linkies, Adolf Heinz; Reuschling, Dieter Bernd

PATENT ASSIGNEE(S): Hoechst Schering AgrEvo GmbH, Germany

SOURCE: Ger. Offen., 23 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|--------------|
| DE 4437137 | A1 | 19960425 | DE 1994-4437137 | 19941018 <-- |
| CA 2202987 | A1 | 19960425 | CA 1995-2202987 | 19951005 <-- |

WO 9611913 A1 19960425 WO 1995-EP3928 19951005 <--
 W: AL, AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP,
 KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL,
 RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN
 RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT,
 LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE,
 SN, TD, TG

AU 9537454 A 19960506 AU 1995-37454 19951005 <--
 EP 787128 A1 19970806 EP 1995-935432 19951005 <--
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE
 CN 1161034 A 19971001 CN 1995-195734 19951005 <--
 BR 9509378 A 19971014 BR 1995-9378 19951005 <--
 HU 77374 A2 19980330 HU 1997-2046 19951005 <--
 JP 10507188 T 19980714 JP 1995-512899 19951005 <--
 IN 1995MA01304 A 20050225 IN 1995-MA1304 19951010 <--
 US 5889012 A 19990330 US 1995-543794 19951016 <--
 ZA 9508749 A 19960513 ZA 1995-8749 19951017 <--

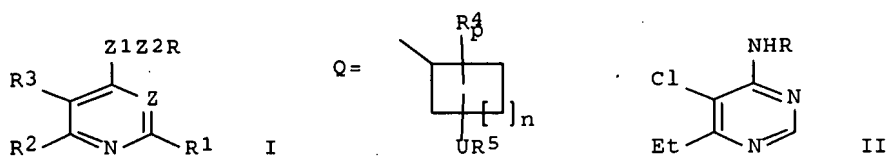
PRIORITY APPLN. INFO.:

DE 1994-4437137 A 19941018 <--
 WO 1995-EP3928 W 19951005 <--

OTHER SOURCE(S): CASREACT 125:33666; MARPAT 125:33666

ED Entered STN: 27 Jun 1996

GI



AB Title compds. [I; R = cycloalkyl group Q; R1 = H, (halo)(cyclo)alkyl; R2,R3 = H, halo, alkyl, alkoxy, etc.; R2R3 = atoms to form a ring; R4 = H, halo, (halo)alkyl, alkoxy, alkylthio; R5 = alk(en)yl, aryl, heterocyclyl, etc.; U = bond, O, SOO-2; Z = CH or N; Z1 = NH, O, SOO-2; Z2 = bond, alkylene; n = 0-4; p = 1 or 2] were prepared. Thus, 4,5-dichloro-6-ethylpyrimidine was aminated by 4-isopropenylcyclohexylamine (predominantly cis) (preparation given) to give title compound II (R = cis-4-isopropenylcyclohexyl) which gave complete kill of Nilaparvata lugens on rice seedlings at 250ppm.

IT 173843-97-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 4-(cycloalkylamino)pyrimidines and analogs as pesticides

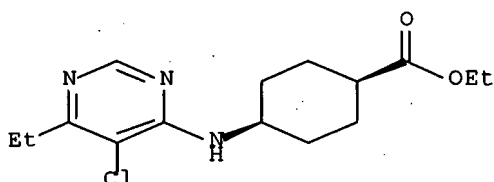
and

agrochem. fungicides)

RN 173843-97-5 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L23 ANSWER 31 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:127981 CAPLUS Full-text

DOCUMENT NUMBER: 124:176139

TITLE: Preparation of pyrimidinylimino- and
-oxocycloalkanecarboxylates and analogs as
agrochemical fungicides and pesticidesINVENTOR(S): Schaper, Wolfgang; Preus, Rainer; Braun, Peter; Knauf,
Werner; Sachse, Burkhard; Waltersdorfer, Anna; Kern,
Manfred; Luemmen, Peter; Bonin, Werner

PATENT ASSIGNEE(S): Hoechst Schering AgrEvo GmbH, Germany

SOURCE: Ger. Offen., 56 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

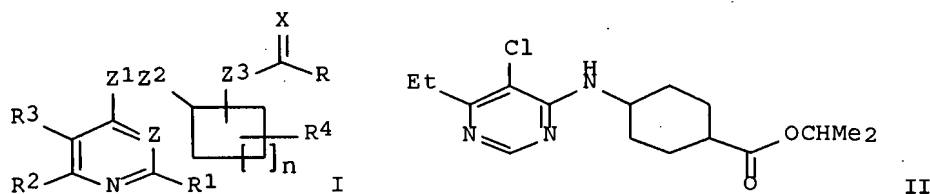
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------------|
| DE 4417163 | A1 | 19951123 | DE 1994-4417163 | 19940517 <-- |
| CA 2190495 | A1 | 19951123 | CA 1995-2190495 | 19950503 <-- |
| WO 9531441 | A1 | 19951123 | WO 1995-EP1666 | 19950503 <-- |
| W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN | | | | |
| RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9525235 | A | 19951205 | AU 1995-25235 | 19950503 <-- |
| AU 703538 | B2 | 19990325 | | |
| EP 759909 | A1 | 19970305 | EP 1995-919376 | 19950503 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE | | | | |
| CN 1148383 | A | 19970423 | CN 1995-193115 | 19950503 <-- |
| BR 9507647 | A | 19970909 | BR 1995-7647 | 19950503 <-- |
| HU 76722 | A2 | 19971028 | HU 1996-3196 | 19950503 <-- |
| JP 10500115 | T | 19980106 | JP 1995-529316 | 19950503 <-- |
| US 5691321 | A | 19971125 | US 1995-441217 | 19950515 <-- |
| ZA 9503957 | A | 19960119 | ZA 1995-3957 | 19950516 <-- |
| PRIORITY APPLN. INFO.: | | | DE 1994-4417163 | A 19940517 <-- |
| | | | WO 1995-EP1666 | W 19950503 <-- |

OTHER SOURCE(S): MARPAT 124:176139

ED Entered STN: 02 Mar 1996

GI

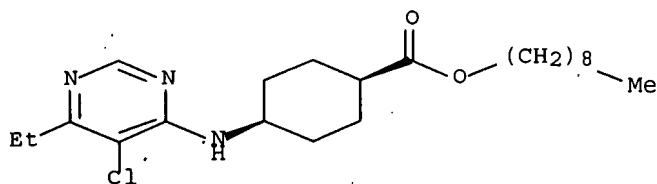


AB Title compds. [I; R = H, OH, alkyl, alkoxy, (di)(alkyl)amino, etc.; R1 = H, halo, (cyclo)alkyl; R2 = H, halo, (cyclo)alkyl, alkoxy, etc.; R3 = H, halo, (halo)alkyl, (halo)alkoxy, etc.; R2R3 = atoms to form a ring; R4 = H, alkyl; X = O or S; Z = CH or N; Z1 = O, S, NH; Z2 = bond, alkylene; Z3 = O, bond; n = 0-5] were prepared. Thus, 4,5-dichloro-6-ethylpyrimidine was aminated by Me cis-4-aminocyclohexanecarboxylate to give, after transesterification, title compound II which gave complete control of Nilaparvata lugens on rice seedlings at 250ppm.

IT 173843-88-4P 173843-89-5P 173843-90-8P
173843-91-9P 173843-92-0P 173843-97-5P
173843-98-6P 173843-99-7P 173844-00-3P
173844-01-4P 173844-02-5P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of pyrimidinylimino- and -oxycycloalkanecarboxylates and analogs as agrochem. fungicides and pesticides)

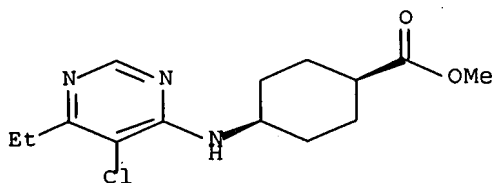
stereochemistry.



RN 173843-88-4 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, methyl ester, cis- (9CI) (CA INDEX NAME)

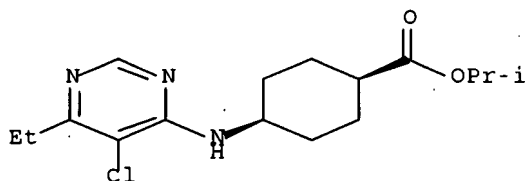
Relative stereochemistry.



RN 173843-89-5 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1-methylethyl ester, cis- (9CI) (CA INDEX NAME)

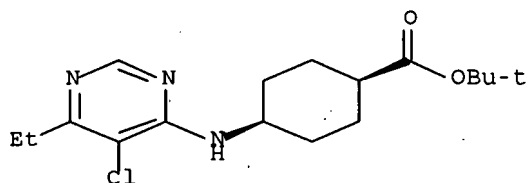
Relative stereochemistry.



RN 173843-90-8 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

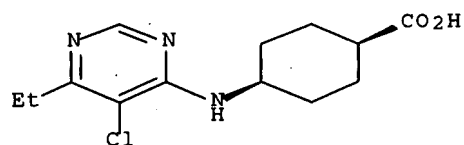
Relative stereochemistry.



RN 173843-91-9 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, cis- (9CI) (CA INDEX NAME)

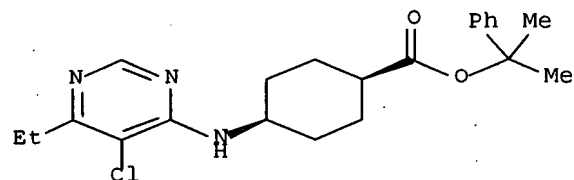
Relative stereochemistry.



RN 173843-92-0 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1-methyl-1-phenylethyl ester, cis- (9CI) (CA INDEX NAME)

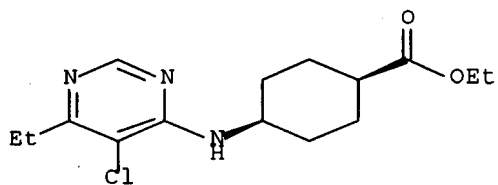
Relative stereochemistry.



RN 173843-97-5 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

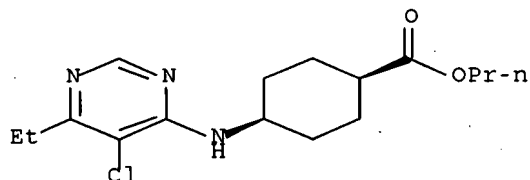
Relative stereochemistry.



RN 173843-98-6 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, propyl ester, cis- (9CI) (CA INDEX NAME)

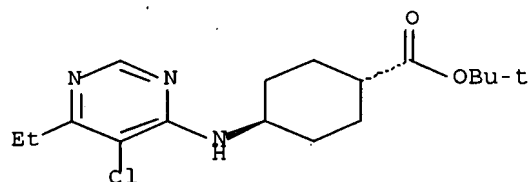
Relative stereochemistry.



RN 173843-99-7 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

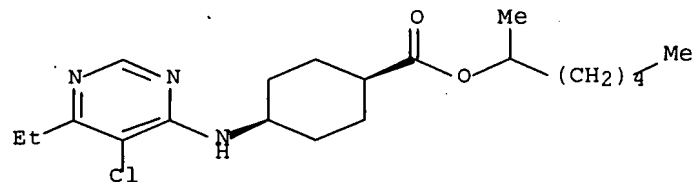
Relative stereochemistry.



RN 173844-00-3 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1-methylhexyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 173844-01-4 CAPLUS

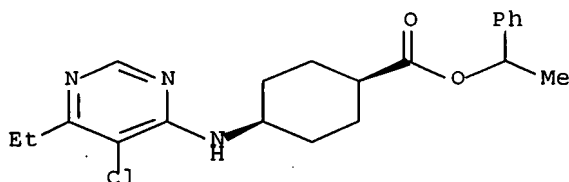
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, nonyl ester, cis- (9CI) (CA INDEX NAME)

Relative

RN 173844-02-5 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1-phenylethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L23 ANSWER 32 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:508815 CAPLUS Full-text

DOCUMENT NUMBER: 121:108815

TITLE: [(Benzodioxane, benzofuran or benzopyran)alkylamino]alkyl-substituted guanidine selective vasoconstrictors

INVENTOR(S): Van Lommen, Guy Rosalia Eugene; De Bruyn, Marcel Frans Leopold; Janssens, Walter Jacobus Joseph

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| WO 9317017 | A1 | 19930902 | WO 1993-EP435 | 19930219 <-- |
| W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO, NZ, PL, PT, RO, RU, SD, SK, UA, US | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG | | | | |
| AU 9334991 | A | 19930913 | AU 1993-34991 | 19930219 <-- |
| AU 664237 | B2 | 19951109 | | |
| EP 639192 | A1 | 19950222 | EP 1993-904017 | 19930219 <-- |
| EP 639192 | B1 | 19960515 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
| JP 07504408 | T | 19950518 | JP 1993-514541 | 19930219 <-- |
| JP 2779268 | B2 | 19980723 | | |
| HU 71129 | A2 | 19951128 | HU 1994-2464 | 19930219 <-- |
| HU 222495 | B1 | 20030728 | | |
| AT 138064 | T | 19960615 | AT 1993-904017 | 19930219 <-- |
| ES 2087721 | T3 | 19960716 | ES 1993-904017 | 19930219 <-- |
| CZ 282092 | B6 | 19970514 | CZ 1994-2020 | 19930219 <-- |
| PL 174736 | B1 | 19980930 | PL 1993-304902 | 19930219 <-- |
| RU 2121999 | C1 | 19981120 | RU 1994-41210 | 19930219 <-- |
| SK 280166 | B6 | 19990910 | SK 1994-1029 | 19930219 <-- |
| RO 115630 | B1 | 20000428 | RO 1994-1432 | 19930219 <-- |
| CA 2117483 | C | 20010109 | CA 1993-2117483 | 19930219 <-- |

| | | | | |
|------------|----|----------|----------------|--------------|
| CN 1079470 | A | 19931215 | CN 1993-103671 | 19930226 <-- |
| CN 1038032 | B | 19980415 | | |
| ZA 9301404 | A | 19940826 | ZA 1993-1404 | 19930226 <-- |
| LT 3049 | B | 19941025 | LT 1993-367 | 19930226 <-- |
| LV 10715 | B | 19951220 | LV 1993-149 | 19930226 <-- |
| IL 104868 | A | 19980104 | IL 1993-104868 | 19930226 <-- |
| US 5541180 | A | 19960730 | US 1994-256995 | 19940729 <-- |
| FI 9403928 | A | 19940826 | FI 1994-3928 | 19940826 <-- |
| FI 109122 | B1 | 20020531 | | |
| NO 9403186 | A | 19940829 | NO 1994-3186 | 19940829 <-- |
| NO 306255 | B1 | 19991011 | | |
| US 5607949 | A | 19970304 | US 1996-632227 | 19960415 <-- |
| US 5624952 | A | 19970429 | US 1996-632226 | 19960415 <-- |
| US 5688952 | A | 19971118 | US 1996-632228 | 19960415 <-- |
| US 5703115 | A | 19971230 | US 1996-632230 | 19960415 <-- |

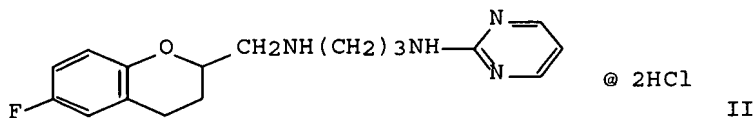
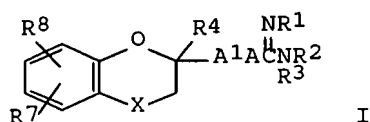
PRIORITY APPLN. INFO.:

| | | |
|----------------|----|--------------|
| US 1992-842560 | A2 | 19920227 <-- |
| WO 1993-EP435 | A | 19930219 <-- |
| US 1994-256995 | A3 | 19940729 <-- |

OTHER SOURCE(S): CASREACT 121:108815; MARPAT 121:108815

ED Entered STN: 03 Sep 1994

GI



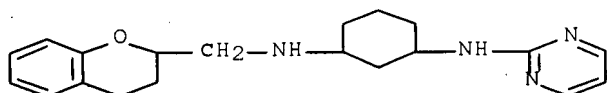
AB The title compds. [I; A = bivalent radical; A1 = bivalent C1-3 alkanediyl radical; R1, R3, R4 = H, C1-6 alkyl; R2 = H, C1-6 alkyl, C3-6 alkenyl, C3-6 alkynyl; R7, R8 = H, halogen, C1-6 alkyl, OH, C3-6 alkenyl, C3-6 alkynyl, CN, CO2H, (un)substituted NH2; X = O, CH2, direct bond], which have selective vasoconstrictor activity, are prepared and I-containing formulations presented. Thus, dihydrochloride salt II was prepared (m.p. 139.9°) and demonstrated 50% of the constrictive response obtained with serotonin upon pig basilar arteries at 1.46 ± 10^{-7} M concentration

IT 155429-41-7P 155429-48-4P

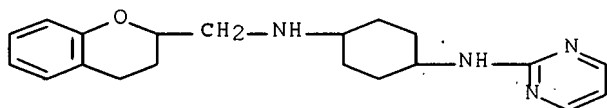
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and selective vasoconstrictor activity of)

RN 155429-41-7 CAPLUS

CN 1,3-Cyclohexanediamine, N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-2-pyrimidinyl- (9CI) (CA INDEX NAME)



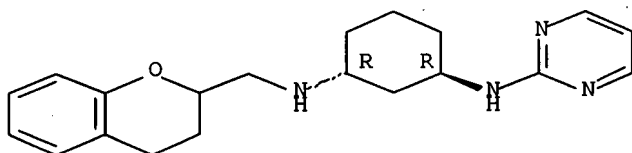
RN 155429-48-4 CAPLUS
 CN 1,4-Cyclohexanediamine, N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-2-pyrimidinyl- (9CI) (CA INDEX NAME)



IT 155426-33-8P 155426-34-9P 155426-39-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 155426-33-8 CAPLUS
 CN 1,3-Cyclohexanediamine, N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-2-pyrimidinyl-, dihydrochloride, trans- (9CI) (CA INDEX NAME)

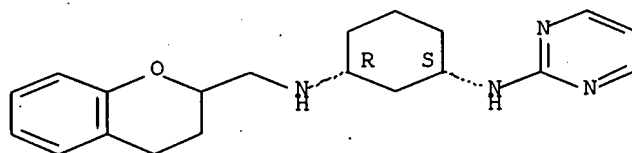
Relative stereochemistry.



● 2 HCl

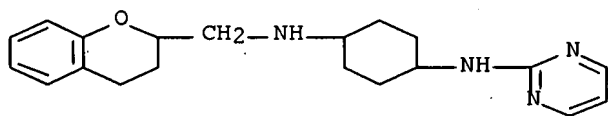
RN 155426-34-9 CAPLUS
 CN 1,3-Cyclohexanediamine, N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-2-pyrimidinyl-, dihydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● 2 HCl

RN 155426-39-4 CAPLUS
 CN 1,4-Cyclohexanediamine, N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-2-pyrimidinyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L23 ANSWER 33 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:431103 CAPLUS Full-text
DOCUMENT NUMBER: 115:31103
TITLE: Polyfunctional reactive dyes
INVENTOR(S): Herd, Karl Josef; Henk, Hermann; Stoehr, Frank Michael
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Eur. Pat. Appl., 105 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------------|------|------------------|-----------------|-----------------|
| EP 395951 | A1 | 19901107 | EP 1990-107503 | 19900420 <-- |
| EP 395951 | B1 | 19940824 | | |
| R: CH, DE, FR, GB, LI | | | | |
| DE 3914628 | A1 | 19901115 | DE 1989-3914628 | 19890503 <-- |
| JP 02308864 | A | 19901221 | JP 1990-115335 | 19900502 <-- |
| US 5274083 | A | 19931228 | US 1991-724443 | 19910702 <-- |
| PRIORITY APPLN. INFO.: | | | DE 1989-3914628 | A 19890503 <-- |
| | | | US 1990-511129 | B1 19900419 <-- |
| OTHER SOURCE(S): | | MARPAT 115:31103 | | |
| ED Entered STN: 27 Jul 1991 | | | | |
| GI | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title dyes 1 [A = direct bond, divalent (cyclo)aliphatic bridging group, divalent aromatic aliphatic bridging group; D1, D2 = direct bond, divalent bridging group; G = chromophoric residue; R,R1,R2 = H, (un)substituted C1-4 alkyl; X = CH:CH₂, CH₂CH₂Y; Y = alkyl-cleavable substituent; Y1 = F, Cl, Br; Z = fiber-reactive residue], useful for dyeing or printing hydroxyl or amide group-containing fabrics, are prepared. Thus, 1-aminoethyl-3-sulfomethyl-4-methyl-6-hydroxy-2-pyridone was condensed with cyanuric chloride, the condensate condensed with ethylenediamine, 5-chloro-2,4,6-trifluoropyrimidine added, and the intermediate coupled with diazotized 2-amino-6-(β -sulfatoethylsulfonyl)-1-naphthalenesulfonic acid forming II which dyed cotton fabrics fast greenish yellow shades.

IT 134559-60-7

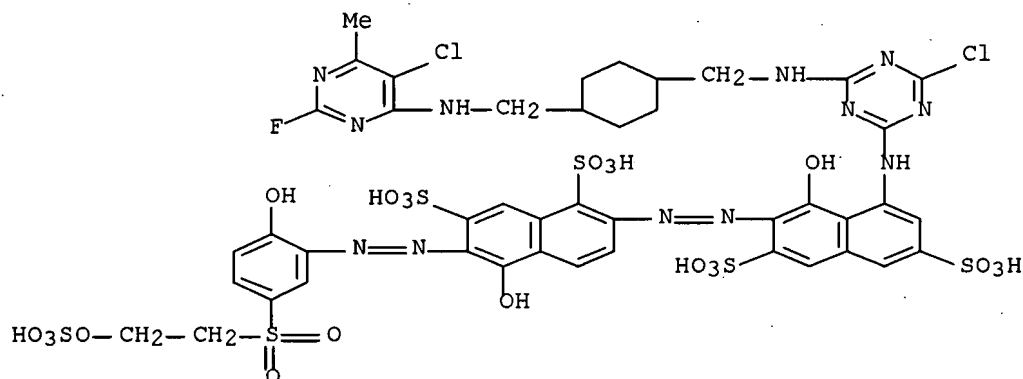
RL: USES (Uses)

(complexation of, with cupric sulfate)

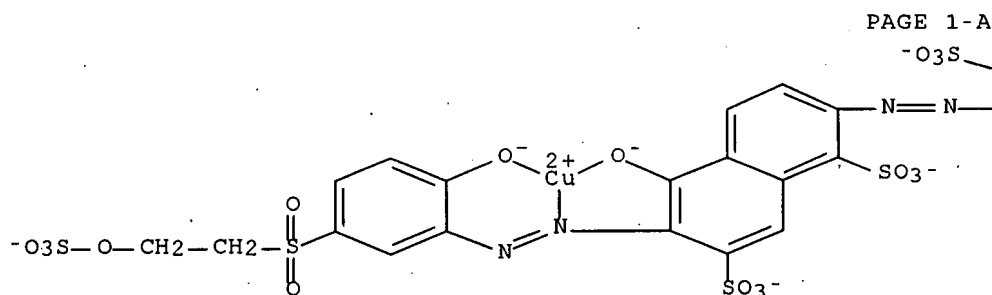
RN 134559-60-7 CAPLUS

CN 1,7-Naphthalenedisulfonic acid, 2-[[8-[[4-chloro-6-[[[4-[[[5-chloro-2-

fluoro-6-methyl-4-pyrimidinyl)amino]methyl]cyclohexyl]methyl]amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]-5-hydroxy-6-[[2-hydroxy-5-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)

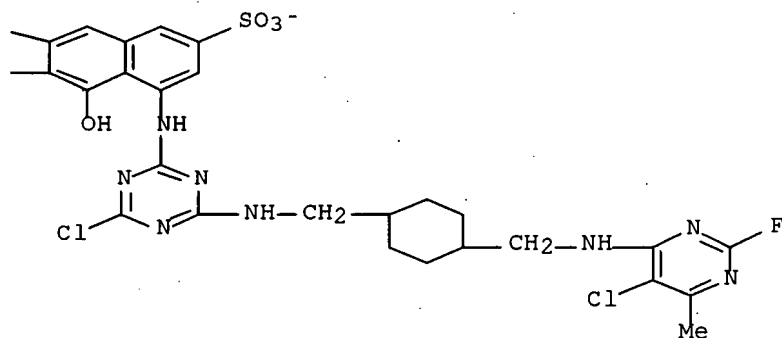


IT 134659-57-7P
 RL: PREP (Preparation)
 (manufacture of, as reactive dye)
 RN 134659-57-7 CAPLUS
 CN Cuprate(5-), [2-[[8-[[4-chloro-6-[[[4-[[[5-chloro-2-fluoro-6-methyl-4-pyrimidinyl)amino]methyl]cyclohexyl]methyl]amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]-5-hydroxy-6-[[2-hydroxy-5-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]-1,7-naphthalenedisulfonato(7-)]-, pentahydrogen (9CI) (CA INDEX NAME)



● 5 H⁺

PAGE 1-B



IT 134559-59-4P 134591-45-0P

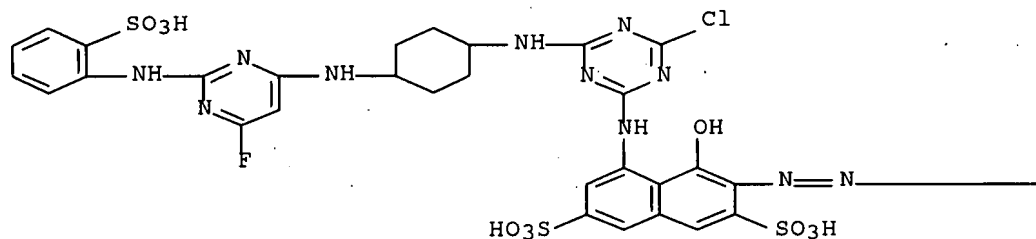
RL: PREP (Preparation)

(manufacture of, as red reactive dye)

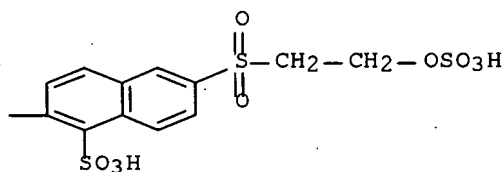
RN 134559-59-4 CAPLUS

CN 2,7-Naphthalenedisulfonic acid, 5-[[4-chloro-6-[[4-[[6-fluoro-2-[(2-sulfophenyl)amino]-4-pyrimidinyl]amino]cyclohexyl]amino]-1,3,5-triazin-2-yl]amino]-4-hydroxy-3-[[1-sulfo-6-[[2-(sulfooxy)ethyl]sulfonyl]-2-naphthalenyl]azo]- (9CI) (CA INDEX NAME)

PAGE 1-A



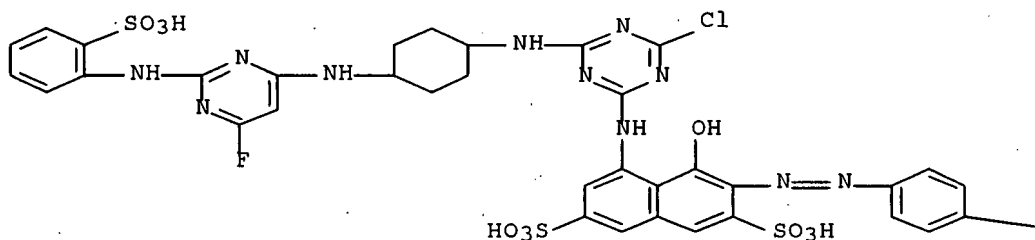
PAGE 1-B



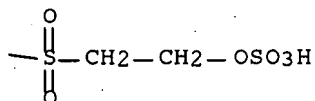
RN 134591-45-0 CAPLUS

CN 2,7-Naphthalenedisulfonic acid, 5-[[4-chloro-6-[[4-[[6-fluoro-2-[(2-sulfophenyl)amino]-4-pyrimidinyl]amino]cyclohexyl]amino]-1,3,5-triazin-2-yl]amino]-4-hydroxy-3-[[4-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)

PAGE 1-A



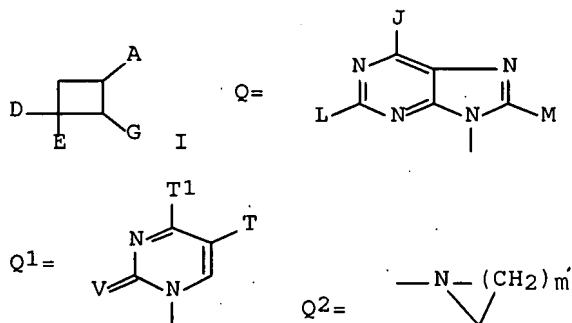
PAGE 1-B



L23 ANSWER 34 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1990:612577 CAPLUS Full-text
 DOCUMENT NUMBER: 113:212577
 TITLE: Preparation of nucleoside cyclobutane analogs as
 antiviral and antitumor agents
 INVENTOR(S): Norbeck, Daniel W.; Plattner, Jacob J.; Rosen, Terry
 J.; Pariza, Richard J.; Sowin, Thomas J.; Garmaise,
 David L.; Hannick, Steven M.
 PATENT ASSIGNEE(S): Abbott Laboratories, USA
 SOURCE: Eur. Pat. Appl., 115 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------------|
| EP 366059 | A2 | 19900502 | EP 1989-119703 | 19891024 <-- |
| EP 366059 | A3 | 19911218 | | |
| R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| CA 2001318 | A1 | 19900425 | CA 1989-2001318 | 19891024 <-- |
| DK 8905292 | A | 19900426 | DK 1989-5292 | 19891024 <-- |
| AU 8943785 | A | 19900503 | AU 1989-43785 | 19891025 <-- |
| JP 03047169 | A | 19910228 | JP 1989-278337 | 19891025 <-- |
| US 5153352 | A | 19921006 | US 1990-570198 | 19900820 <-- |
| US 5246931 | A | 19930921 | US 1991-694538 | 19910501 <-- |
| PRIORITY APPLN. INFO.: | | | US 1988-262547 | A 19881025 <-- |
| | | | US 1989-319385 | A 19890303 <-- |
| | | | US 1989-420691 | A 19891017 <-- |

OTHER SOURCE(S): MARPAT 113:212577
 ED Entered STN: 08 Dec 1990
 GI



AB The title compds. [I; A = purin-9-yl (Q), pyrimidin-1-yl (Q1) or its heterocyclic isostere; J, L = H, OH, alkoxy, SH, thioalkoxy, N3, Q2, (un)substituted NH2, N:CHNH2, NHOH, or NHNH2; m = 1-6; M = H, alkyl, halo, Q2, (un)substituted NH2; T = H, alkyl, 2-haloethyl, halomethyl, CF2H, CF3, halo, cyano, NO2, CH:CH2, SH, NHOH, unsubstituted NH2, Q2, etc.; V = O, S; T1 = OH, SH, alkoxy, thioalkoxy, halo, Q2; D, G = H, alkyl, OH, CH2OH, alkoxymethyl, alkylcarbonyloxymethyl, aminoalkylcarbonyloxymethyl, etc.; E = H, CH2OH, OH;] are prepared Thus, condensation of 2,3- bis(hydroxymethyl)cyclobutylamine hydrochloride with 2-amino-4,6- dichlorpyrimidine in EtOH containing Et3N and diazo coupling of the resulting 3-[(2'-amino-6'-chloro-4'-pyrimidinyl)amino]-1,2- bis(hydroxymethyl)cyclobutane with 4-ClC6H4N2+Cl- followed by Zn reduction in AcOH gave 3-[(6'-chloro-2',5'-diamino-4'-pyrimidinyl)amino]-1,2- bis(hydroxymethyl)cyclobutane. Cyclocondensation of the latter with AcOCH2(OEt)2 under reflux followed by hydrolysis gave 9-[2',3'- bis(hydroxymethyl)cyclobutyl]guanine (II). Approx. 25 I were prepared and II in vitro was active against herpes simplex virus, human immunodeficiency virus 1 and 2, human cytomegalovirus, and Varicella-Zoster virus. II in vivo was active against hepatitis B virus in ducklings and HIV in mice. II and 4 other I showed antitumor activity against human lung carcinoma A549, human adenocarcinoma HCT-8 and mouse lymphocytic leukemia P388-DI.

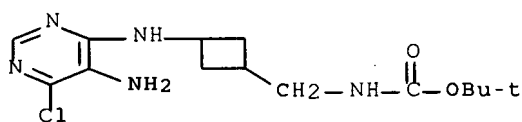
IT 130369-11-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for carbocyclic nucleoside cyclobutane analog)

RN 130369-11-8 CAPLUS

CN Carbamic acid, [[3-[(5-amino-6-chloro-4-pyrimidinyl)amino]cyclobutyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1980:34951 CAPLUS Full-text

DOCUMENT NUMBER: 92:34951

TITLE: Correlation analysis of pyrimidine folic acid antagonists as antibacterial agents. I.

AUTHOR(S): Coats, Eugene A.; Genther, Clara S.; Smith, Carl C.

CORPORATE SOURCE: Coll. Pharm., Univ. Cincinnati, Cincinnati, OH, 45267, USA

SOURCE: European Journal of Medicinal Chemistry (1979), 14(3), 261-70

CODEN: EJMCA5; ISSN: 0009-4374

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

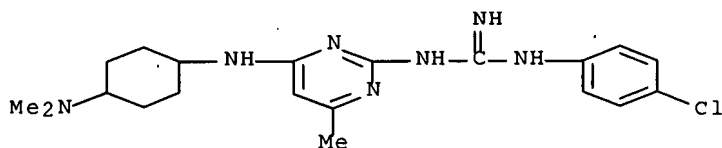
AB The activities of 175 pyrimidines as inhibitors of *Streptococcus faecium*, *Lactobacillus casei*, and *Pediococcus cerevisiae* are reported. In addition, the mode of action according to the ability of folic acid [59-30-3] or folinic acid [58-05-9] to reverse the inhibitory effect of the pyrimidines was determined. The 2,4-diamino substituent pattern appeared to be the dominant but not the sole factor controlling mode of action. Quant. structure-activity relations using regression anal., substituent consts., and indicator variables were developed in an effort to delineate influences on potency and to quant. differences between the test systems. Although aromatic and(or) lipophilic substituents at the 5 position of 2,4-diaminopyrimidines enhanced folate reversible inhibition against all 3 systems the derived equations quant. establish differences in and limitations on the extent of this effect.

IT 51386-71-1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(bactericidal activity of, structure in relation to)

RN 51386-71-1 CAPLUS

CN Guanidine, N-(4-chlorophenyl)-N'-[4-[[4-(dimethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



L23 ANSWER 36 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1974:103776 CAPLUS Full-text

DOCUMENT NUMBER: 80:103776

TITLE: Antimalarial drugs. 35. Synthesis and antimalarial effects of 1-(3,4-dichlorophenyl)-3-[4-[(1-ethyl-3-piperidyl)amino]-6-methyl-2-pyrimidinyl]guanidine and related substances

AUTHOR(S): Elslager, Edward F.; Werbel, Leslie M.; Curry, Ann; Headen, Nancy; Johnson, Judith

CORPORATE SOURCE: Res. Dev. Div., Parke, Davis and Co., Ann Arbor, MI, USA

SOURCE: Journal of Medicinal Chemistry (1974), 17(1), 75-100

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

AB Structure-antimalarial activity of 1-(3,4-dichlorophenyl)-3-[4-[(1-ethyl-3-piperidyl)amino]-6-methyl-2-pyrimidinyl]guanidine (I) [21062-28-2] and 120 analogs prepared by condensation of the aryl(4-chloro-6-methyl-2-pyrimidinyl)guanidine derivs. with the appropriate polyamines is given. Curative activity against Plasmodium berghei infection in mice was shown by 90 compds. in single s.c. doses of 20-640 mg/kg. While 62 compds showed suppressive activity after oral administration, 46 of them were 2-30 times as potent as quinine-HCl [130-89-2]. Strong suppressive activity against P. gallinaceum in chicks was shown by 59 compds.

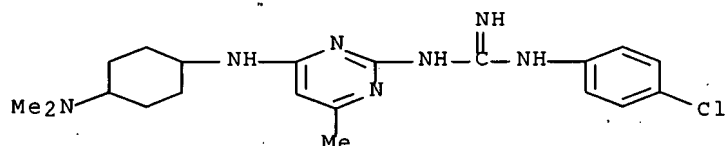
IT 51386-71-1P 51386-99-3P 51387-03-2P

51387-45-2P 51387-46-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and antimalarial activity of)

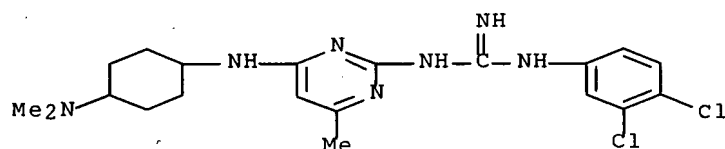
RN 51386-71-1 CAPLUS

CN Guanidine, N-(4-chlorophenyl)-N'-[4-[[4-(dimethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



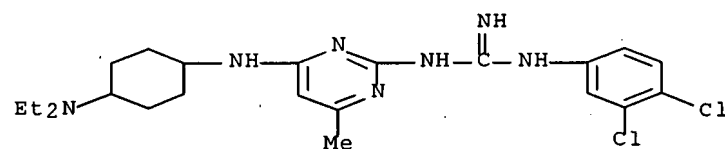
RN 51386-99-3 CAPLUS

CN Guanidine, N-(3,4-dichlorophenyl)-N'-[4-[[4-(dimethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



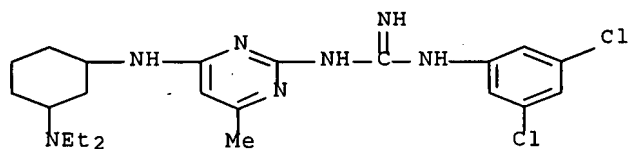
RN 51387-03-2 CAPLUS

CN Guanidine, N-(3,4-dichlorophenyl)-N'-[4-[[4-(diethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



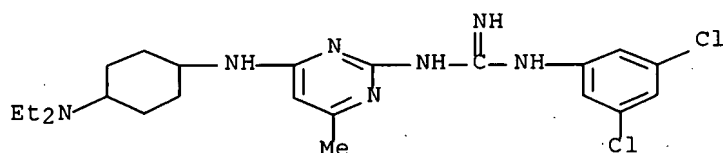
RN 51387-45-2 CAPLUS

CN Guanidine, N-(3,5-dichlorophenyl)-N'-[4-[[3-(diethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 51387-46-3 CAPLUS

CN Guanidine, N-(3,5-dichlorophenyl)-N'-[4-[[4-(diethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)



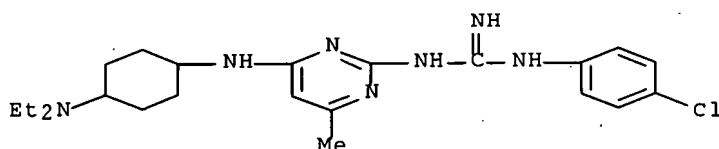
● HCl

IT 51386-73-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51386-73-3 CAPLUS

CN Guanidine, N-(4-chlorophenyl)-N'-[4-[[4-(diethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



L23 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1973:478734 CAPLUS Full-text

DOCUMENT NUMBER: 79:78734

TITLE: Synthesis and antimalarial effects of
5,6-dichloro-2-[[4-[[4-(diethylamino)-1-
methylbutyl]amino]-6-methyl-2-
pyrimidinyl]amino]benzimidazole and related
benzimidazoles and 1H-imidazo[4,5-b]pyridines

AUTHOR(S): Werbel, Leslie M.; Curry, Ann; Elslager, Edward F.;
Hess, Carolyn

CORPORATE SOURCE: Res. Dev. Div., Parke, Davis and Co., Ann Arbor, MI,
USA

SOURCE: Journal of Heterocyclic Chemistry (1973),
10(3), 363-82

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

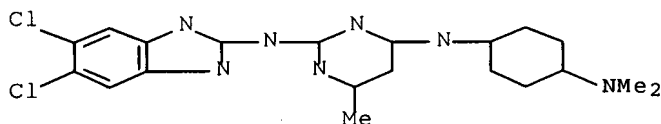
AB Fifty-five 2-[[4-[(dialkylamino)alkyl]amino]-6-methyl-2-pyrimidinyl]amino]benzimidazoles were prepared in 3-88% yields by the condensation of the requisite 2-[(2-benzimidazolyl)amino]-4-chloro-6-methylpyrimidine with the appropriate polyamine in EtOH-HCl or neat with excess amine containing KI. The 2-[(2-benzimidazolyl)amino]-6-methyl-4-pyrimidinol precursors, obtained in 11-51% yields by cyclization of 2-(cyanoamino)-4-hydroxy-6-methylpyrimidine with a suitably substituted o-phenylenediamine, were chlorinated with POCl₃ to give the intermediate 2-[(2-benzimidazolyl)amino]-4-chloro-6-methylpyrimidines (27-99%). Oxidation of 5,6-dichloro-2-[[4-[(4-(diethylamino)-1-methylbutyl]amino]-6-methyl-2-pyrimidinyl]amino]benzimidazole with m-chloroperbenzoic acid gave the distal N4'-oxide (19%). Fusion of 2,3-diaminopyridine with 2-(cyanoamino)-4-hydroxy-6-methylpyrimidine provided 2-[(4-hydroxy-6-methyl-2-pyrimidinyl)amino]-1H-imidazo[4,5-b]pyrimidine (30%), which upon chlorination with POCl₃ (63%) followed by amination with N,N-diethylethylenediamine afforded 2-[4-[[2-(diethylamino)ethyl]amino]-6-methyl-2-pyrimidinyl]-1H-imidazo[4,5-b]pyridine (8%). Thirty-eight 2-[(4-amino-6-methyl-2-pyrimidinyl)amino]benzimidazoles possessed curvative activity against Plasmodium berghei at single subcutaneous doses ranging from 20-640 mg/kg. Orally, 31 compds. exhibited suppressive activity against P. berghei comparable with or superior to the reference drugs 1-(p-chlorophenyl)-3-[4-[[2-(diethylamino)ethyl]amino]-6-methyl-2-pyrimidinyl]guanidine (I) and quinine-HCl while 12 of them were 5 to 28 times as potent as I and quinine-HCl. Eight compds. also displayed strong suppressive activity against P. gallinaceum in chicks. 5,6-Dichloro-2-[[4-[2-(diethylamino)ethyl]amino]-6-methyl-2-pyrimidinyl]-benzimidazole showed marked activity against a cycloguanil-resistant line of P. berghei, and the most promising member of the series, i.e. 5,6-dichloro-2-[[4-[[4-(diethylamino)-1-methylbutyl]amino]-6-methyl-2-pyrimidinyl]amino]benzimidazole (I), was designated for preclinical toxicol. studies and clin. trial. Structure-activity relations are discussed.

IT 42388-86-3P 42388-91-0P 42388-92-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 42388-86-3 CAPLUS

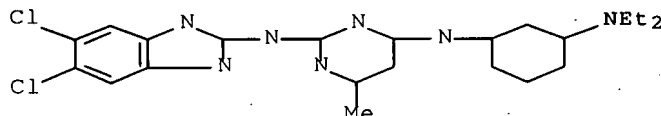
CN 2,4-Pyrimidinediamine, N2-(5,6-dichloro-1H-benzimidazol-2-yl)-N4-[4-(dimethylamino)cyclohexyl]-6-methyl- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 42388-91-0 CAPLUS

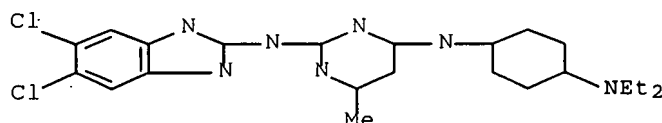
CN 2,4-Pyrimidinediamine, N2-(5,6-dichloro-1H-benzimidazol-2-yl)-N4-[3-(diethylamino)cyclohexyl]-6-methyl- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 42388-92-1 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(5,6-dichloro-1H-benzimidazol-2-yl)-N4-[4-(diethylamino)cyclohexyl]-6-methyl- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L23 ANSWER 38 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1972:60924 CAPLUS Full-text

DOCUMENT NUMBER: 76:60924

TITLE: Fiber-reactive dyes

INVENTOR(S): Bien, Hans S.; Klauke, Erich

PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.

SOURCE: Brit. Amended, 75 pp.

CODEN: BSXXAH

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|----------------|
| GB 1169254 | A | 19700811 | GB 1967-40774 | 19670906 <-- |
| PRIORITY APPLN. INFO.: | | | DE 1966-F50181 | A 19660910 <-- |
| | | | DE 1967-F51942 | A 19670325 <-- |

ED Entered STN: 12 May 1984

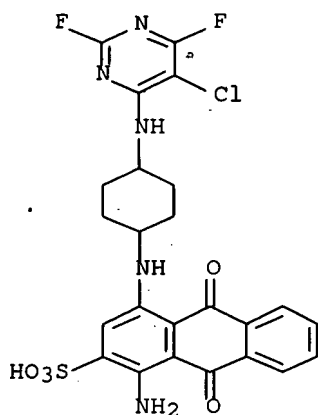
AB The title chlorodifluoropyrimidine dyes (I; R = H, Me; Q = anthraquinone, azo, metal complex azo, nitro, or Cu phthalocyanine dye residue), useful for dyeing cellulose and wool wetfast shades, were prepared by treating amino dyes with 5-chloro-2,4,6-trifluoropyrimidine (II). For example, diazotized 2-aminonaphthalene-4,8-disulfonic acid was coupled with m-toluidine, the azo dye dissolved in water, Me₂CO and NaOH added, and the mixture treated with II at 20-30.deg. and pH 5.5-6 to give 2-[4-(5-chloro-2,6-difluoro-4-pyrimidinylamino)-o-tolylazo]naphthalene-4,8-disulfonic acid [34086-94-7], printing cellulose fabric wash- and lightfast reddish yellow. Similarly, 65 other I were prepared

IT 35434-62-9P

RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)

RN 35434-62-9 CAPLUS

CN 2-Anthracenesulfonic acid, 1-amino-4-[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]cyclohexyl]amino]-9,10-dihydro-9,10-dioxo- (9CI) (CA INDEX NAME)



L23 ANSWER 39 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1970:68209 CAPLUS Full-text

DOCUMENT NUMBER: 72:68209

TITLE: Fiber-reactive dyes

INVENTOR(S): Bien, Hans S.; Oertzen, Klaus V.; Harms, Wolfgang

PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.

SOURCE: Brit., 9 pp.

CODEN: BRXXAA

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|--------------|
| GB 1170195 | | 19691112 | GB 1968-10879 | 19680306 <-- |
| DE 1644614 | | | DE | |
| PRIORITY APPLN. INFO.: | | | DE | 19670325 <-- |

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

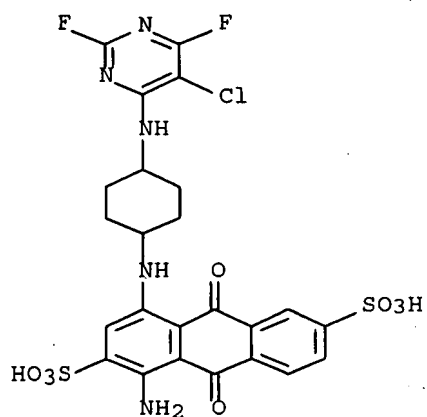
AB Compds. of the general formula I dye wool and cotton blue. Thus, 10.8 parts 1-amino-4-(4-aminocyclohexylamino)anthraquinone-2,6-disulfonic acid dissolved in 115 parts H₂O was acylated at 0-5° with 3.7 parts 2,4,6-trifluoro-5-chloropyrimidine at pH 9-10, maintaining this pH with 2N NaOH, adjusted to pH 5.5 with HCl, and treated with 6 parts NaCl to precipitate I [R₁ = R₃ = H, R₂ = SO₃H, Y = Y₁ (X = F)]. Similarly, other I were prepared (R₁-R₃ and Y given): H, SO₃H, H, Y₁ (X = Cl); H, SO₃H, H, Y₂ (Z = CO); H, SO₃H, H, Y₂ (Z = SO₂); H, H, SO₃H, Y₁ (X = F); SO₃H, H, H, Y₁ (X = F).

IT 24460-66-0P 25980-28-3P 25980-29-4P
25980-32-9P

RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)

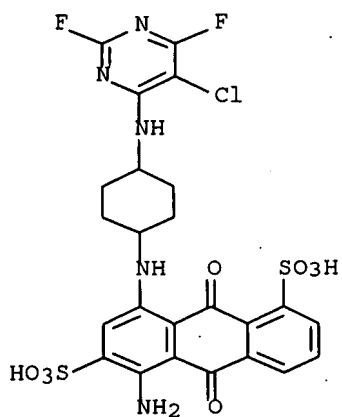
RN 24460-66-0 CAPLUS

CN 2,6-Anthracenedisulfonic acid, 1-amino-4-[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]cyclohexyl]amino]-9,10-dihydro-9,10-dioxo- (8CI) (CA INDEX NAME)



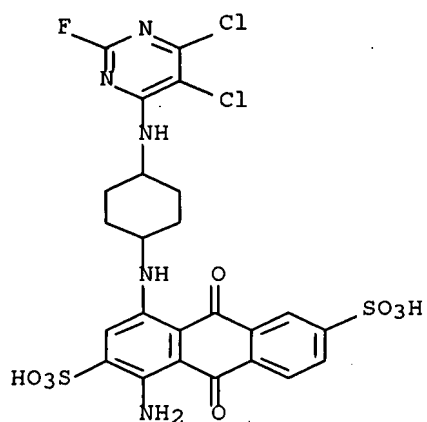
RN 25980-28-3 CAPLUS

CN 1,6-Anthracedisulfonic acid, 5-amino-8-[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]cyclohexyl]amino]-9,10-dihydro-9,10-dioxo- (8CI) (CA INDEX NAME)



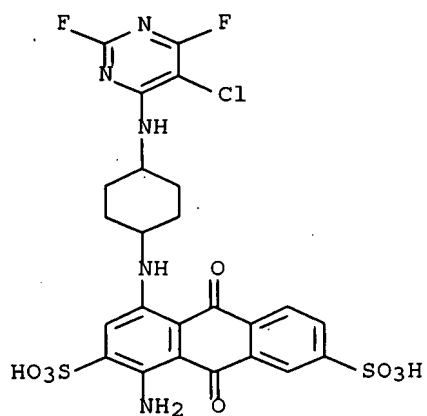
RN 25980-29-4 CAPLUS

CN 2,6-Anthracedisulfonic acid, 1-amino-4-[[4-[(5,6-dichloro-2-fluoro-4-pyrimidinyl)amino]cyclohexyl]amino]-9,10-dihydro-9,10-dioxo- (8CI) (CA INDEX NAME)



RN 25980-32-9 CAPLUS

CN 2,7-Anthracedisulfonic acid, 1-amino-4-[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]cyclohexyl]amino]-9,10-dihydro-9,10-dioxo- (8CI) (CA INDEX NAME)

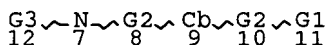
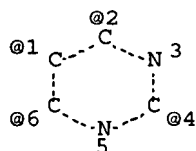


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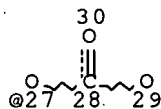
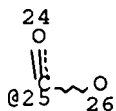
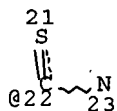
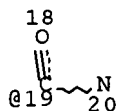
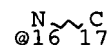
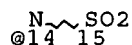
SEARCH HISTORY

=> d stat que l19; d his nofile

L3 STR



Ak @13



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REP G2=(0-1) 13

VAR G3=1/2/4/6

NODE ATTRIBUTES:

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CONNECT IS E2 RC AT 9

CONNECT IS E2 RC AT 13

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY SAT AT 9

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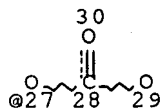
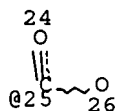
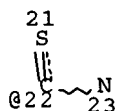
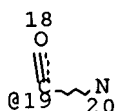
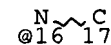
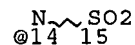
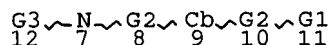
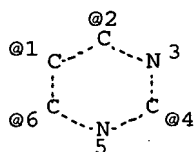
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STEREO ATTRIBUTES: NONE

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L16 STR



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REP G2=(0-4) C

VAR G3=1/2/4/6

NODE ATTRIBUTES:

NSPEC IS RC AT 17

CONNECT IS E2 RC AT 9

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY SAT AT 9

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M4-X7 C AT 9

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L19 3163 SEA FILE=REGISTRY SUB=L9 SSS FUL (L16 AND L3)

100.0% PROCESSED 563914 ITERATIONS

3163 ANSWERS

SEARCH TIME: 00.00.11

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L1 STR
L2 9 SEA SSS SAM L1
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L3 STR L1
L4 9 SEA SSS SAM L3
D SAVED

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E US2004-812075/APPS
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E 46.195.39/RID
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 L10 359 SEA ABB=ON L9 AND L6

FILE 'CAPLUS' ENTERED AT 09:36:01 ON 29 JUN 2007

L11 4 SEA ABB=ON L10
 L12 0 SEA ABB=ON L11 AND (PY<2003 OR AY<2003 OR PRY<2003)

FILE 'REGISTRY' ENTERED AT 09:37:04 ON 29 JUN 2007

L13 575386 SEA ABB=ON DIMETHYLAMINO
 L14 359 SEA ABB=ON L10 AND L13
 L15 13 SEA SUB=L9 SSS SAM L3
 L16 STR L3
 L17 13 SEA SUB=L9 SSS SAM (L16 AND L3)
 D SCAN
 L18 563914 SEA SUB=L9 SSS FUL (L16 AND L3) EXTEND
 L19 3163 SEA SUB=L9 SSS FUL (L16 AND L3)
 SAVE TEMP L19 JAI075FULL/A
 L20 357 SEA ABB=ON L19 AND L10
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FILE 'CAPLUS' ENTERED AT 09:43:11 ON 29 JUN 2007

L22 77 SEA ABB=ON L19
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D STAT QUE L19

FILE 'CAPLUS' ENTERED AT 09:44:18 ON 29 JUN 2007

D QUE NOS L23
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D STAT QUE L19

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